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On the Many-Particle Structure of Green's Functions in Quantum Field Theory

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The structure of the expectation values of retarded multiple commutators (r functions) is analyzed in terms of the number of particles in the decomposition of absorptive parts. As to the one-particle structure, it is found that an r function is a sum of a finite number of terms, each of them except one (that one being called one-particle irreducible) being in momentum space a product of one-particle irreducible factors, linked by one-particle propagation functions. As to the two-particle structure, it is found that a one-particle irreducible function is the solution of an inhomogeneous Bethe-Salpeter equation, whose kernel and inhomogeneous term both are two-particle irreducible functions. This structure, which could be generalized to higher particle numbers, closely resembles perturbation theory but is here derived from locality and the asymptotic condition alone, by converting the nonlinear system of integral equations for r functions stepwise into one in which neither one- or two-particle reducible functions, nor one- or two-particle intermediate states appear. The implication of such structure analysis for an interpretation of perturbation theory, improvements of present methods to derive analytic properties of scattering amplitudes, and a formalism with unstable particles are discussed, and the strength of singularities of various functions investigated.

INTRODUCTION

AXIOMATIC quantum field theory consists in studying the consequences for observable quantities of locality, which means that the commutator (or anticommutator) of any two local quantities, like field operators, should vanish at spacelike distances. It is well known that the most convenient objects to analyze are the vacuum expectation values of certain infinite sets of operator products: unordered products, giving rise to w functions[1]; time-ordered products, giving rise to τ functions[2]; and retarded multiple commutators, giving rise to r functions.[3]

The axioms of the theory, notably relativistic invariance, locality, and the existence of discrete eigenstates of the energy-momentum-squared operator, imply certain properties of those functions. Firstly, there are properties expressible for each function separately, mainly deduced from relativistic invariance and locality, and secondly, properties that relate all those functions together. Of this latter type are the positive definiteness condition for w functions[1] and the infinite systems of coupled nonlinear integral equations for τ[2] and r functions,[4] where specific properties of the state space of the theory are explicitly used.

A great deal of work has recently been done on the first-mentioned "linear" properties. However, it has been shown by Jost[5] that the linear conditions are not sufficient to establish analyticity of the meson-nucleon vertex function in the cut energy-plane. On the other hand, it is known that the nonlinear conditions are important in proofs of dispersion relations for scattering amplitudes. Thus, it seems to be desirable to find out generally what kind of properties of the invariant functions these conditions imply, a question that has received comparatively little attention.

It will be shown that the nonlinear conditions determine the many-particle structure of the functions in

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[1] A. S. Wightman, Phys. Rev. **101**, 860 (1956).

[2] See e.g., H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo cimento **1**, 205 (1955).

[3] See e.g., H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo cimento **6**, 319 (1957).

[4] V. Glaser, H. Lehmann, and W. Zimmermann, Nuovo cimento **6**, 1122 (1957); K. Nishijima, Progr. Theoret. Phys. **17**, 765 (1957).

[5] R. Jost, Helv. Phys. Acta **31**, 263 (1958).

question. Here the r functions are the most convenient ones since their nonlinear system of integral equations is simplest. This is because, in contrast to τ functions, for r functions the locality condition is a linear one: the r functions are to be invariant retarded functions. The nonlinear conditions merely express the absorptive part of an r function as a sum of bilinear terms arising from various intermediate states, the number of particles in those states usually ranging from one to infinity. According to this decomposition of the absorptive parts, the r functions have several types of singularities in momentum space: delta-function-like ones from one-particle intermediate states and discontinuities of the derivatives at the thresholds of many-particle contributions.

To understand the structure of r functions in view of these singularities, one starts best from perturbation theory. This is because the renormalized perturbation theoretical expansion of the r functions is a formal solution of the axiomatic scheme and, actually, the only form of a solution we know at present. Moreover, if one sets out with the aim of finding a formal solution of the scheme as a power series expansion in a perturbation parameter (or set of parameters) one is uniquely led[6] to the renormalized perturbation theoretical expansions compatible with the assumed types of stable particles. Therefore we start, short of something better, from perturbation theory and try to find out those of its features that render it a solution, though a formal one, of the nonlinear system as particularized in the foregoing.

A perturbation theoretical contribution to an r function is described by a double graph.[7] The skeleton of such a graph is the same as that of a Feynman graph. However, there is one distinguished vertex (the latest one) and the lines in the graph do not stand for Δ_F but for Δ_{Ret} and Δ_1 functions. In such a graph one can perform partial summations, as is well known for Feynman graphs as well as for the graphs of the nuclear many-body problem. What we call structure of a graph is the circumstance that there might be one line, or pair of lines, that is the only connection between otherwise disconnected parts of that graph, both parts in themselves having again the skeleton of a most general double graph. There may be, of course, several graph parts that are connected with one another by such simple links.

If no restriction is imposed on the number of legs a vertex in the graph may have and, of course, no restriction on the number of vertices, the structure just described is the most general property that can be abstracted from perturbation theory (apart from the permissible singularities of r functions, which will be discussed later). This structure is exhibited in closed form by requiring the r functions to be solutions of inhomogeneous Bethe-Salpeter equations, where both the kernels and the inhomogeneous terms are irreducible in the sense that their absorptive parts do not have contributions from one, or two, particle intermediate states. This structure is verified by inserting it into the nonlinear system of integral equations, whereupon all one- and two-particle singularities (or reducibilities) drop out and the properties of kernels and inhomogeneous terms just mentioned are manifested.[7a] The key to this phenomenon is the fact explained before, namely that the perturbation theoretical solution, whose structure was taken as a guide, is a formal solution of the nonlinear system. Actually, we shall show that the ansatz chosen by us does not imply a loss of generality at the beginning.

The implication of these findings is two-fold. Firstly, they lead to a new interpretation of perturbation theory as a degenerate form of structure analysis, since irreducibility of vertices, or absence of intermediate states of low mass, means decreased extension in space-time. Secondly, they can be exploited to enlarge the analyticity region of scattering amplitudes, or to prove such analyticity for up to now excluded mass ratios, or possibly, to find new analytic properties for which the nonlinear conditions are crucial.

One feature of renormalizable perturbation theory not taken into account is the estimate of the strength of singularities, or growth at infinity in momentum space, of each single term of the expansion. In accordance with our earlier admitting "unrenormalizable" vertices, we believe perturbation theory not to be indicative here, and actually to be too generous, as is already known for special cases,[8] and we shall collect arguments for that opinion. Further study of the consistency of the suitably reduced nonlinear system should give an answer to this question as well to others that arise from the, in comparison with perturbation theory, here widened viewpoint.

In the first part generalized retarded functions are introduced as formal tools for later use.

In the second part the one-particle singularities of retarded functions are studied in some detail, mainly to display the method used in the more complicated analysis of two-particle singularities in the third part, details of which are deferred to an appendix.

In the fourth part these results are generalized to higher singularities, and their implications for an interpretation of perturbation theory are discussed.

The strength of singularities of propagation and vertex functions is discussed in the fifth part, with an appendix containing calculational details.

The final part gives an outlook on possible applications of the formalism to the specific problem of analytic continuation of scattering amplitudes. These applica-

[6] R. Haag, Kgl. Danske Videnskab. Selskab, Mat. fys. Medd. 29, 12 (1955). The question of renormalization was cleared up in the paper cited in footnote 2.

[7] F. J. Dyson, Phys. Rev. 82, 428 (1951).

[7a] At this point our proof is not yet complete, though a very indicative result is obtained.

[8] H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo cimento 2, 425 (1955).

tions will be dealt with further in a later paper. Also it is shown what meaning the concept, or use, of unstable particles may have in the present scheme.

1. GENERALIZED RETARDED FUNCTIONS

We shall discuss in nearly all of the following a theory with one hermitian scalar field $A(x)$, obeying

$$[A(x),A(y)]=0 \quad \text{if} \quad (x-y)^2<0, \tag{1}$$

and one kind of neutral spinless particles only. The extension of all results to more realistic cases is straightforward.

A convenient tool to handle infinite sets of functions or operators are generating functionals. They are generally not supposed to exist in any other than a formal sense, provided each function or operator of that infinite set exists. The generating functional of time ordered operator products

$$T(x_1\cdots x_n)=\sum_{\text{perm}}\theta(x_1-x_2)\cdots\theta(x_{n-1}-x_n) \times A(x_1)\cdots A(x_n) \tag{2}$$

is the operator

$$\mathcal{T}\{J\}=1+\sum_{n=1}^{\infty}\frac{i^n}{n!}\int\cdots\int dx_1\cdots dx_n T(x_1\cdots x_n) \times J(x_1)\cdots J(x_n), \tag{3}$$

where $J(x)$ is a source function that plays an algebraic role only.[9] We shall abbreviate

$$\mathcal{T}\{J\}\equiv\mathcal{T}, \quad \frac{\delta^n\mathcal{T}\{J\}}{\delta J(x_1)\cdots\delta J(x_n)}\equiv\mathcal{T}_{1\ldots n},$$

the J dependence being understood.

The use of $\mathcal{T}$ presupposes that the products (2) are well defined. As we shall see, it suffices to this end that the vacuum expectation values be well defined. We defer the discussion of this restriction to a later section and will be satisfied for the moment with the deliberate restriction to theories where the singularities of vacuum expectation values of operator products are not worse than in each perturbation theoretical order of renormalizable theories, which implies the existence of the vacuum expectation values of time ordered products and retarded commutators as tempered distributions for which moreover all operations carried out in this section are well defined and orders of integrations can be freely interchanged. A thorough discussion of this latter point has recently been given by Zimmermann.[10] *Note added in proof.*—(To Sec. 1.) The solution presented in Eq. (25) holds formally (i.e., in the power series expansion and apart from ultraviolet difficulties, which do not show up in the formal manipulations), if the interaction is switched off at large positive and negative times, whereby relativistic invariance in the large is destroyed. The Green's functions with $J\neq 0$, however, correspond to a situation where the term $J(x)A(x)$, with $A(x)$ as always the renormalized field, is added to the Lagrangian density. Thus, existence of the usual Green's functions with $J\equiv 0$ (in the sense of no need of subtractions, cf. the beginning of Sec. 1) can be interpretated as "measurability" of the renormalized field even when the amplitude renormalization is infinite.—From the c number property of the commutator $[A_{in}(x),A_{in}(y)]$ it follows that integrations of the type Eqs. (13), (14), or (17) and of the type (15) can be interchanged among themselves, but not with each other. (Integrations of the type (16) can be interchanged with both other types.) The noninterchangeability disappears for "reduced" functionals that are obtained from the original ones in an analogous way as φ functions were obtained from τ functions in the reference of footnote 2 and does not affect the later calculations. (To Sec. 2) Eq. (48) is not a consequence of (47), and $\psi(\bar{u},\bar{v})=0$ is not the only solution of (59), if $\tilde{\Delta}_{\text{Ret}}'(p)$ has zeros, because here for the process of amputation the retarded boundary condition, which made the amputation unique till here, is no longer available. The additional terms $\tilde{\psi}(p)=i\pi\epsilon(p_0)\sum c_\lambda\delta(x_\lambda-p^2)$, which give rise to the CDD zeros as seen in Eq. (102), cannot be thought to be contained in the term written in Eq. (49) because delta functions are not absolute squares. NonCDD zeros are excluded if the restriction mentioned at the beginning of Sec. 1 is invoked, as follows from the result of Appendix B. (To Sec. 3.) The phenomenon explained in the foregoing note is expected to show up also here because of the distinct analogy between the one- and the two-particle structure analysis. This means that though the inverse $1-F_i'$ of $1+F'$ in Eq. (73) is still unique provided the retarded boundary condition is applicable it can be expected that nontrivial solutions X^i, Y^i, $Z^i\neq 0$ of Eqs. (80) ff will remain, analogous to CDD R functions. Of course, this does not imply that an ambiguity will necessarily persist if the analysis is carried further.—The author is indebted to Dr. S. Mandelstam for having pointed out to him the perturbation theoretical example of an unstable particle, which suggests X^i, Y^i, $Z^i\neq 0$. (To Sec. 4.) The remarks presented under A on the relation of structure analysis to a theory with field equations, like quantum electrodynamics, stand amplification. If there is a subtraction permitted for the vertex, a nonvanishing dispersive part (namely, a constant) is compatible with a vanishing absorptive part of the vertex that is two-particle irreducible with respect to an external coordinate. If no subtraction is made, the dispersive part would also

[9] The functional $\mathcal{T}\{J\}$, being unitary, might have a more than formal meaning. If we do not, in all of the following, set $J=0$ after a finite number of differentiations, but keep it finite, we obtain reducible and irreducible Green's functions in the presence of an external source, like an external current in quantum electrodynamics; see footnote 18a. Schwinger (footnote 18) introduced that functional this way.

[10] W. Zimmermann, Nuovo cimento **10**, 597 (1958) and forthcoming paper.

vanish, which leads to vanishing results throughout. (The dispensability of a subtraction follows similarly as in Sec. 5 for the original vertex, because the Born approximation is the same. These considerations do not apply to a superrenormalizable theory where in general the Born approximation of the vertex does not vanish.)

It is well known that because of (1) and the present remarks, $\mathcal{T}$ transforms relativistically[11] according to[12]

$$U(a,\Lambda)\mathcal{T}\{J\}U(a,\Lambda)^{-1}=\mathcal{T}\{J'\}, \tag{4}$$

where $J'(x)=J(a+\Lambda x)$. Since $\mathcal{T}$ can be written

$$\mathcal{T}\{J\}=T\exp\left(i\int A(x)J(x)dx\right),$$

it is unitary:

$$\mathcal{T}^+\mathcal{T}=\mathcal{T}\mathcal{T}^+=1. \tag{5}$$

We now introduce the functional of two source functions

$$\mathfrak{R}\{\bar{J},J\}=\mathcal{T}^+\{J+i\bar{J}/2\}\mathcal{T}\{J-i\bar{J}/2\}, \tag{6}$$

which generates an infinite set of operator products depending on two sets of coordinates,

$$R(x_1\cdots x_m,y_1\cdots y_n)=\frac{\delta^{m+n}}{\delta\bar{J}(x_1)\cdots\delta\bar{J}(x_m)\delta J(y_1)\cdots\delta J(y_n)}\mathfrak{R}\{\bar{J},J\}\mid_{\bar{J}=J=0}. \tag{7}$$

We shall use the abbreviations,

$$\mathfrak{R}\{\bar{J},J\}\equiv\mathfrak{R},$$

$$\frac{\delta^{m+n}}{\delta\bar{J}(x_1)\cdots\delta\bar{J}(x_m)\delta J(x_{m+1})\cdots\delta J(x_{m+n})}\mathfrak{R}\{\bar{J},J\}\equiv\mathfrak{R}_{1\cdots m,m+1\cdots m+n} \tag{8}$$

as well as

$$\mathfrak{R}_{1\cdots m,m+1\cdots m+n\mid\bar{J}=0}\equiv R_{1\cdots m,m+1\cdots m+n}.$$

Since $\mathfrak{R}$ is hermitean[13] and transforms in analogy to Eq. (4), the products in Eq. (7) are hermitean and their vacuum expectation values,

$$\langle R(x_1\cdots x_m,y_1\cdots y_n)\rangle\equiv r(x_1\cdots x_m,y_1\cdots y_n),$$

are real relativistically invariant functions (distributions).

From (5) and (6) we find

$$R_x=-i\mathcal{T}^+\mathcal{T}_x=i\mathcal{T}_x{}^+\mathcal{T}, \tag{8}$$

which shows that R_x is the generating functional of the usual retarded multiple commutators,[14] which obeys

$$R_{x,y}=i\theta(x-y)[R_x,R_y]. \tag{9}$$

Especially, we have

$$[R_x,R_y]=0 \quad \text{if} \quad (x-y)^2<0 \tag{10}$$

as a generalization of (1). From (6) and (8) we find

$$R_{1\ldots m}=2^{1-m}\sum_{\text{perm}}\theta(x_1-x_2)\cdots\theta(x_{m-1}-x_m)\times\{\cdots\{\{R_1,R_2\},R_3\},\cdots R_m\}. \tag{11}$$

Thus, for exclusively spacelike distances among the x we have

$$R_{12\ldots m}=R_1R_2\cdots R_m.$$

Therefore, these products are the many-time generalization of products introduced by Nishijima.[15,16] From (9) and (11) follows that they vanish unless each y in (7) is timelike advanced with respect to at least one x:

$$R_{x_1\cdots x_m,y}=0 \quad \text{unless} \quad y<x_\nu, \quad \nu\epsilon 1\cdots m. \tag{12}$$

The x, however, are not subject to any restriction, apart from that following from Eq. (12).

From (11) and the well-known reduction formula[17] for retarded commutators,

$$[A_{\text{in}}(y),R_x]=i\int dz\Delta(y-z)\mathbf{K}_zR_{x,z},$$

where $\mathbf{K}_z=\partial_z{}^\mu\partial_{z\mu}+m^2$, or directly from the asymptotic condition and (6), (8) we find

$$[A_{\text{in}}(y),\mathfrak{R}_x]=i\int dz\Delta(y-z)\mathbf{K}_z\mathfrak{R}_{x,z}. \tag{13}$$

In order to deduce the expansion of $\mathfrak{R}$ in normal-ordered products, we insert the general ansatz,

$$\mathfrak{R}=:\exp\left[\int duA_{\text{in}}(u)\mathbf{K}_u\delta/\delta J'(u)\right]:F\{\bar{J},J,J'\}\mid_{J'=0},$$

where F is a c number functional into (13). This leads to

$$\int dz\Delta(y-z)\mathbf{K}_z[\delta/\delta J(z)-\delta/\delta J'(z)]F\{\bar{J},J,J'\}=0$$

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[11] We use standard notations; see e.g., footnote 1.

[12] Equations like (4) and following ones mean that upon expansion of both sides in powers of J the symmetrized coefficients of each order on both sides are equal, or that equality holds upon functionally differentiating both sides any number of times and then setting J identically zero. See, however, footnote 9.

[13] The remarks in footnote 9 apply to this functional in an analogous sense, because of its close relation to $\mathcal{T}\{J\}$, at least for purely imaginary $\bar{J}$ and for the derivatives $R_{1\ldots m}$.

[14] See footnotes 3, 4. Retarded products were already used by G. Källén and J. C. Polkinghorne.

[15] K. Nishijima, footnote 4. See also K. Baumann, Z. Physik **152**, 448 (1958).

[16] They are not, however, related to products recently introduced by J. C. Polkinghorne, Proc. Roy. Soc. (London) **A247**, 557 (1958), which would be deduced from the generating functional $\mathcal{T}^+\{J\}\mathcal{T}\{J+\bar{J}\}\mathcal{T}^+\{\bar{J}\}$.

[17] W. Zimmermann, Nuovo cimento **10**, 597 (1958). For instance, let $y_0\to-\infty$ in (9). In convolutions the Klein-Gordon operator $\mathbf{K}$ will always stand next to a solution or Green's function of the Klein-Gordon equation and operates on the other factor, be it to the right or left.

provided J' is on the mass shell, and therefore allows to replace in the foregoing equation $\delta/\delta J'(u)$ by $\delta/\delta J(u)$. Upon identification of $F\{\bar{J},J,0\}$ by taking the vacuum expectation value, we obtain the desired expansion

$$\mathfrak{R}=:\exp\left[\int du A_{\text{in}}(u)\mathbf{K}_u\delta/\delta J(u)\right]:\langle\mathfrak{R}\rangle. \quad (14)$$

We furthermore find directly from (6) and the asymptotic condition,

$$\mathfrak{R}_x=\frac{1}{2}\{A_{\text{in}}(x),\mathfrak{R}\}+\int du\Delta_{\text{Ret}}(x-u)\mathbf{K}_u\mathfrak{R}_u \quad (15)$$

and

$$\mathfrak{R}_{x,y}=\int du\Delta_{\text{Av}}(y-u)\mathbf{K}_u\mathfrak{R}_{x,u} \quad (16)$$

and for the boundary term in Eq. (15),

$$\frac{1}{2}\{A_{\text{in}}(y),\mathfrak{R}_x\}=A_{\text{in}}^{(-)}(y)\mathfrak{R}_x+\mathfrak{R}_xA_{\text{in}}^{(+)}(y)+\frac{1}{2}\int du\Delta_1(y-u)\mathbf{K}_u\mathfrak{R}_{x,u}. \quad (17)$$

Equation (15) is obviously the generalization of the usual

$$R_x=A_{\text{in}}(x)+\int du\Delta_{\text{Ret}}(x-u)\mathbf{K}_uR_u. \quad (15a)$$

From (6) various identities between the generalized retarded products can be derived. Keeping in mind the retardedness described in (12) we are only interested in identities not involving step functions. They are obtained from (6) by repeated differentiation and use of (5), (8). We list those relations we shall need later:

$$R_{x,y}-R_{y,x}=i[R_x,R_y], \quad (18)$$

$$R_{xy}=\frac{1}{2}\{R_x,R_y\}, \quad (19)$$

$$R_{xy,z}=\frac{1}{2}\{R_{z,x},R_y\}+\frac{1}{2}\{R_{z,y},R_x\}+i[R_{xy},R_z], \quad (20)$$

$$R_{xyz}=-\frac{1}{4}R_{z,xy}+\frac{1}{2}\{R_{xy},R_z\}+\frac{i}{4}[R_{z,x},R_y]+\frac{i}{4}[R_{z,y},R_x]. \quad (21)$$

A nonrecursive formula for a general $R_{xyz}\cdots$ can also be derived. Another set of identities is obtained from

$$\mathfrak{R}\{\bar{J},J\}\mathfrak{R}\{-\bar{J},J\}=1$$

upon differentiation, which gives an especially simple expression for $R_{xyz}\cdots$ with an even number of first indices in terms of lower $R_{uvw}\cdots$.

The generalized retarded products with not more than n first indices provide simple expressions for the scattering amplitudes for processes with $n+1$ outgoing and an arbitrary number of ingoing particles. Namely, from (6) and (14) we find

$$(-i)^n\mathcal{T}^+\mathcal{T}_{1\cdots n}=:\exp\left[\int du A_{\text{in}}(u)\mathbf{K}_u\delta/\delta J(u)\right]:\cdot\left(\delta/\delta\bar{J}_1-\frac{i}{2}\delta/\delta J_1\right)\cdots\left(\delta/\delta\bar{J}_n-\frac{i}{2}\delta/\delta J_n\right)\langle\mathfrak{R}\rangle|_{\bar{J}=0}.$$

From this, the matrix element

$$\langle\text{one particle}|T(x_1\cdots x_n)|\text{ ingoing particles}\rangle,$$

and thus the desired scattering amplitude is immediately found.

We shall later draw conclusions from the structure of the perturbation theoretical expansion of $\mathfrak{R}\{\bar{J},J\}$, which we therefore derive here in an entirely formal manner, disregarding all questions of existence and renormalization terms. Let the field equation be

$$\mathbf{K}_xA(x)=-H_w'[A(x)].$$

Then Schwinger's functional differential equation[18] becomes

$$-i\mathbf{K}_x\mathcal{T}_x=-H_w'[-i\delta/\delta J(x)]\mathcal{T}+J(x)\mathcal{T}. \quad (22)$$

From Eq. (22), the hermitean conjugate equation, and Eq. (6) we find

$$\mathbf{K}_x\mathfrak{R}_x=-\left(\frac{1}{2}H_w'\left[\delta/\delta\bar{J}(x)-\frac{i}{2}\delta/\delta J(x)\right]+\frac{1}{2}H_w'\left[\delta/\delta\bar{J}(x)+\frac{i}{2}\delta/\delta J(x)\right]\right)\mathfrak{R}+J(x)\mathfrak{R} \quad (23)$$

and

$$\mathbf{K}_y\mathfrak{R}_{x,y}=\left\{-iH_w'\left[\delta/\delta\bar{J}(y)-\frac{i}{2}\delta/\delta J(y)\right]+iH_w'\left[\delta/\delta\bar{J}(y)+\frac{i}{2}\delta/\delta J(y)\right]\right\}\mathfrak{R}_x+\bar{J}(y)\mathfrak{R}_x. \quad (24)$$

The conversion into integral equations[18a] could be

[18] J. Schwinger, Proc. Natl. Acad. Sci. 37, 452 (1951). See also N. N. Bogoliubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields* (Interscience Publishers, Inc., New York, 1959), p. 424. We shall refer to this book as *B* and *S*.

[18a] These integral equations lead, upon expansion in powers of $\bar{J}$ and J, to two infinite systems of coupled linear integral equations between r functions that stand to double graphs in the same relation as the infinite system of integral equations for r functions obtained from the integrated form of (22) stands

done according to (15) and (16). The formal solution of (23), (24) can be found with the help of functional Fourier transforms,[19] or by insertion of the well-known formal solution of (22),

$$\mathcal{T}=S^+:\exp\left[\int duA_{\text{in}}(u)\mathbf{K}_u\delta/\delta J(u)\right]:$$
$$\cdot\exp\left(-i\int H_w[-i\delta/\delta J(x)]dx\right)$$
$$\cdot\exp\left[-\frac{1}{2}\int\int dydy'J(y)\Delta_F(y-y')J(y')\right]$$

into (6). The result is

$$\mathfrak{R}\{\tilde{J},J\}=:\exp\left[\int duA_{\text{in}}(u)\mathbf{K}_u\delta/\delta J(u)\right]:$$
$$\cdot\exp\left(-\int H_w'[\delta/\delta\tilde{J}(x)]\delta/\delta J(x)dx+(2^2\cdot 3!)^{-1}\right.$$
$$\left.\times\int H_w'''[\delta/\delta\tilde{J}(x)]\delta^3/\delta J(x)^3dx-+\cdots\right)$$
$$\cdot\exp\left[\frac{1}{4}\int\int dydz\tilde{J}(y)\Delta_1(y-z)\tilde{J}(z)\right.$$
$$\left.+\int\int dydz\tilde{J}(y)\Delta_{\text{Ret}}(y-z)J(z)\right], \quad (25)$$

which can also directly be checked to be a solution of (23), (24). The structure implied by (25) will later be investigated. For the moment we only remark that expanding (25) gives rise to the "double graphs" described by Dyson.[20,21]

As remarked in the introduction, R_x as found from (25) is also a formal solution of the basic equation (9) as is not difficult to check. Moreover, the structure of the renormalized perturbation theoretical solution, which is the unique solution of (9) in the precise perturbation theoretical sense, is the same as that derivable from (25) if H_w is properly chosen and self energies and vertex parts are summed up.

2. ONE-PARTICLE STRUCTURE

The one-particle singularities of Feynman amplitudes have recently been investigated by Zimmermann.[22] He found that on the basis of locality and the asymptotic condition alone, these singularities can be proved to be those one infers from a general Feynman graph.

We first derive a similar result for r functions, closely following Zimmermann's method.

Define

$$R_{\text{out}}(x;\eta_1\cdots\eta_r)$$
$$\equiv R(x,x+\eta_1\cdots x+\eta_r)$$
$$-\int dx'\Delta_{\text{Av}}(x-x')\mathbf{K}_{x'}R(x',x'+\eta_1\cdots x'+\eta_r). \quad (26)$$

According to Zimmermann,[23] the Fourier transform of this operator is proportional to that of the operator $A_{\text{out}}(x)$. Because of the generating functional (8) of retarded commutators we have by partial integration,

$$R(x,x+\eta_1\cdots x+\eta_r z_1\cdots z_s)$$
$$=\int dx'\Delta_{\text{Av}}(x-x')\mathbf{K}_{x'}R(x',x'+\eta_1\cdots z_s)$$
$$+\frac{\delta^s}{\delta J(z_1)\cdots\delta J(z_s)}$$
$$\times[\mathcal{T}^+\{J\}R_{\text{out}}(x;\eta_1\cdots\eta_r)\mathcal{T}\{J\}]|_{J=0} \quad (27)$$

and

$$R(x,x+\eta_1\cdots x+\eta_r z_1\cdots z_s)$$
$$=\int dx'\Delta_{\text{Ret}}(x-x')\mathbf{K}_{x'}R(x',x'+\eta_1\cdots z_s). \quad (28)$$

With the definition

$$\int dxe^{ipx}R_{\text{out}}(x;\eta_1\cdots\eta_r)$$
$$\equiv(2\pi)^{\frac{1}{2}}\delta(p^2-m^2)R_{\text{out}}(p;\eta_1\cdots\eta_r),$$

we obtain for the Fourier transforms of (27) and (28),

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to Feynman graphs. The equations are the covariant form of the system of coupled integral equations found by W. Zimmermann, Nuovo cimento 11, 577 (1954). The advanced functional $\mathcal{T}\{J-(i/2)\tilde{J}\}\mathcal{T}^+\{J+(i/2)\tilde{J}\}$ also satisfies (23), (24), but obeys different boundary conditions. The role of J as a source is seen from (8), (22), (15a), which give $R_x=A_{\text{in}}(x)+\int du\Delta_{\text{Ret}}(x-u)[-H_w'(R_u)+J(u)]$.

[19] See e.g., B and S, p. 484.

[20] F. J. Dyson, footnote 7. See also C. N. Yang and D. Feldman, Phys. Rev. 79, 972 (1950) and G. Källén, Arkiv Fysik 2, 371 (1950).

[21] If (25) is expanded, it leads to graphs with vertices that are connected by any odd number of advanced lines to later vertices, and not only by one such line as in Dyson's description. This is because of the fact that in (25) the $i\Delta^+$ and $-i\Delta^-$ lines arising in the Heisenberg representation approach have been split into Δ_1 and Δ lines, and the latter lines been absorbed among the Δ_{Ret} lines, taking into account all possible distributions of lines on a given skeleton. The simplest example is provided by two parallel contraction lines between two points: $i\Delta^+\cdot i\Delta^+ + (-i\Delta^-)\cdot(-i\Delta^-) = 2^{-1}\Delta_1\cdot\Delta_1 - 2^{-1}\Delta\cdot\Delta = 2^{-1}\Delta_1\cdot\Delta_1 - 2^{-1}\Delta_{\text{Ret}}\cdot\Delta_{\text{Ret}} - 2^{-1}\Delta_{\text{Av}}\cdot\Delta_{\text{Av}}$. Note also (11).

[22] W. Zimmermann, Nuovo cimento 13, 503 (1959).

[23] W. Zimmermann, Nuovo cimento 10, 567 (1958), where a proof is given for time-ordered products. By using the results of R. Haag, Phys. Rev. 112, 669 (1958), however, the proof can be extended to R products.

$$R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)$$
$$=[(p-i\epsilon)^2-m^2]^{-1}[(p^2-m^2)R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)]$$
$$+(2\pi)^{\frac{1}{2}}\delta(p^2-m^2)\frac{\delta^s}{\delta J(z_1)\cdots\delta J(z_s)}$$
$$\times[\mathcal{T}^+\{J\}R_{\text{out}}(p;\eta_1\cdots\eta_r)\mathcal{T}\{J\}]|_{J=0}$$
$$=[(p+i\epsilon)^2-m^2]^{-1}[(p^2-m^2)R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)].$$

In the difference

$$2\pi i\epsilon(p_0)\delta(p^2-m^2)[(p^2-m^2)R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)]$$
$$=(2\pi)^{\frac{1}{2}}\delta(p^2-m^2)\frac{\delta^s}{\delta J(z_1)\cdots\delta J(z_s)}$$
$$\times[\mathcal{T}^+\{J\}R_{\text{out}}(p;\eta_1\cdots\eta_r)\mathcal{T}\{J\}]|_{J=0},$$

we insert, because of the above remark,

$$\delta(p^2-m^2)R_{\text{out}}(p;\eta_1\cdots\eta_r)$$
$$=\delta(p^2-m^2)R_{\text{out}}(p)C(p;\eta_1\cdots\eta_r),$$

where $C(p;\eta_1\cdots\eta_r)$ is a c number, such that

$$2\pi i\epsilon(p_0)\delta(p^2-m^2)[(p^2-m^2)R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)]$$
$$=(2\pi)^{\frac{1}{2}}\delta(p^2-m^2)\frac{\delta^s}{\delta J(z_1)\cdots\delta J(z_s)}$$
$$\times[\mathcal{T}^+\{J\}R_{\text{out}}(p)\mathcal{T}\{J\}]|_{J=0}C(p;\eta_1\cdots\eta_r).$$

The omission of $\eta_1\cdots\eta_r$ permits, because of $C(p)=1$, to eliminate R_{out}. This gives

$$\delta(p^2-m^2)[(p^2-m^2)R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)]$$
$$=\delta(p^2-m^2)[(p^2-m^2)R(p;z_1\cdots z_s)]C(p;\eta_1\cdots\eta_r).$$

In order to eliminate $C(p;\eta_1\cdots\eta_r)$, we keep only $z_1=0$ and take the vacuum expectation value. Because of

$$-(p^2-m^2)\langle R(p;0)\rangle=\int dx e^{ipx}\mathbf{K}_x\Delta_R'(x)dx=1$$

if $p^2=m^2$ we finally obtain[24]

$$\delta(p^2-m^2)[(p^2-m^2)R(p;\eta_1\cdots\eta_r,z_1\cdots z_s)]$$
$$=-\delta(p^2-m^2)[(p^2-m^2)R(p;\eta_1\cdots\eta_r,0)]$$
$$\times[(p^2-m^2)R(p;z_1\cdots z_s)], \quad (29)$$

where also an integration over $\eta_1\cdots\eta_r$ should be performed.

For the following, we wish to generalize (29), returning to functionals. To this end it is convenient to derive from (25) a one-particle-structure ansatz which conforms with (29) for each possible singularity.

Consider the most general double graph[20] in the perturbation expansion of (25). Since the skeleton is the same as that of a Feynman graph, all interior and end lines will be self-energy corrected, and thus actually be the function,

$$r(x,y)=\Delta_{\text{Ret}}'(x-y)=i\theta(x-y)\langle[A(x),A(y)]\rangle$$

for retarded and

$$\tfrac{1}{2}\Delta_1'(x-y)=\tfrac{1}{2}\langle\{A(x),A(y)\}\rangle$$

for contraction lines. These latter lines, however, will not appear explicitly in the following.

Next, note that the expansion of the functional $\langle R_x\rangle$ is

$$\langle R_x\rangle=\int dz\Delta_{\text{Ret}}'(x-z)J(z)+\langle R_x'\rangle, \quad (30)$$

where $\langle R_x'\rangle$ contains the second and higher powers of J and will, due to (15a) and the remarks just made, begin with a Δ_{Ret}'-function at x. We shall find it sometimes useful to display it by writing

$$\langle R_x'\rangle=\int dz\Delta_{\text{Ret}}'(x-z)\langle R_z'\rangle,$$

where barring a coordinate means "amputation" by division in momentum space.[25] Similarly, from (16) and the foregoing remarks, we infer the presence of Δ_{Av}' lines at the coordinates at which, according to (7), J is attached. Altogether we have

$$\langle R_x'\rangle=\sum_{n=2}^{\infty}\frac{1}{n!}\int\cdots\int dz du_1\cdots du_n dv_1\cdots dv_n\Delta_{\text{Ret}}'(x-z)$$
$$\times\langle R(\bar{z},\bar{u}_1\cdots\bar{u}_n)\rangle\cdot\Delta_{\text{Ret}}'(u_1-v_1)$$
$$\times J(v_1)\cdots\Delta_{\text{Ret}}'(u_n-v_n)J(v_n),$$

and correspondingly,

$$\langle R_{\bar{x},1\cdots\bar{n}}'\rangle$$
$$=\langle R(\bar{x},\bar{y}_1\cdots\bar{y}_m)\rangle$$
$$+\sum_{n=1}^{\infty}\frac{1}{n!}\int\cdots\int dv_1\cdots dv_n\langle R(\bar{x},\bar{y}_1\cdots\bar{y}_m\bar{u}_1\cdots\bar{u}_n)\rangle$$
$$\times\Delta_{\text{Ret}}'(u_1-v_1)J(v_1)\cdots\Delta_{\text{Ret}}'(u_n-v_n)J(v_n). \quad (31)$$

We shall now use a graphical notation where the last functional is represented by a circle, a smaller circle on the periphery denoting the (amputated) first coordinate, and the function Δ_{Ret}' is represented by a barred double line.

From (25) one easily sees that a line that connects two otherwise separated graph parts must be a retarded or, more precisely, Δ_{Ret}' line, and that both those parts are again the most general double graphs with the re-

[24] Equation (29) is analogous to Eq. (35) of footnote 22; K. Nishijima, footnote 4, and K. Baumann, footnote 15, give in the last factor on the right-hand side of (29) the time-ordered product.

[25] The question of zeros of $\tilde{\Delta}_{\text{Ret}}'(p)$ will be discussed in detail in Sec. 5 and will be seen to present no difficulty here.

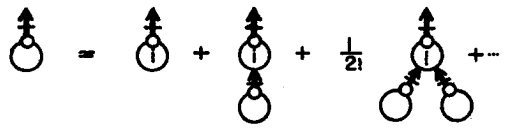

FIG. 1. General one-particle structure of $\langle R_x' \rangle$, Eq. (33).

maining external lines and the new external line at the bridge. This fact, well known for Feynman graphs, is due to the exponential structure of (25). However, if all integrations should be over all space-time, the later graph part should be one-particle irreducible between the latest coordinate x and the bridge to avoid double counting, but will in general have one-particle bridges to other graph parts. Thus the general structure we conjecture to be correct is the generalization of (31) shown in Fig. 1 which, as explained in the foregoing, stands for the functional equation,

$$\langle R_x' \rangle = \langle R_x{}^i \rangle + \sum_{n=1}^{\infty} \frac{1}{n!} \langle R_{x,\bar{1}\ldots\bar{n}}{}^i \rangle \langle R_1' \rangle \cdots \langle R_n' \rangle \quad (32)$$

where integration over repeated coordinates is implied. The functional $\langle R_x{}^i \rangle$, whose further indices indicate functional derivatives as usual, is supposed to be one-particle irreducible between any two coordinates being displayed as well as those being set free by further functional differentiation. The precise meaning of this condition will soon become clear.

It is important to note that (32) does not imply a loss of generality, because it can be solved for $\langle R_x{}^i \rangle$ by iteration of

$$\langle R_x{}^i \rangle = \langle R_x' \rangle + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \langle R_{x,\bar{1}\ldots\bar{n}}' \rangle \langle R_1{}^i \rangle \cdots \langle R_n{}^i \rangle, \quad (33)$$

obtained from (32), or

$$\langle R_x'\{J\} \rangle = \langle R_x{}^i\{\hat{J}\} \rangle$$

with

$$\hat{J}(x) = J(x) + \langle R_{\bar{x}}'\{J\} \rangle = \langle R_{\bar{x}}\{J\} \rangle = J(x) + \langle R_{\bar{x}}{}^i\{\hat{J}\} \rangle. \quad (34)$$

To any finite order m of J, the sums and iterative solution of (33) break off. Thus, no convergence problems are here involved,[26] and (33) defines the functional $\langle R_x{}^i \rangle$ explicitly. The same breakoff takes place in (32). With (33) it is not difficult to show that $\langle R_x{}^i \rangle$ is not one-particle singular, in the sense of (29), with respect to any separation of its coordinates into two groups.

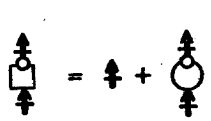

FIG. 2. Decomposition of $\langle R_{x,y} \rangle$, Eq. (37).

[26] Such problems could arise if the functionals were used non-formally, see footnotes 9 and 13.—The author is indebted to Dr. H. Araki for having pointed out that an earlier form of (33), (34) was incorrect.

Equations (33) and (34) display that $\langle R_x{}^i \rangle$ is again a real invariant retarded functional in the sense of (12). It is this convenient separation of retardedness (12) and completeness (18) that renders the retarded functions suitable for our analysis. As we shall see, in the two-particle structure analysis (12) has also to be used at later steps of the argument.

We now use the abbreviation,

$$\langle R_{x,uv\ldots}{}^{is} \rangle \equiv \langle R_{x,uv\ldots}{}^{i} \rangle + \sum_{n=1}^{\infty} \frac{1}{n!} \langle R_{x,\bar{1}\ldots\bar{n}uv\ldots}{}^{i} \rangle \langle R_1' \rangle \cdots \langle R_n' \rangle. \quad (35)$$

Therefore, the indices of $\langle R_x{}^{is} \rangle$ do not mean functional derivatives. Instead, we have

$$\frac{\delta}{\delta J(y)} \langle R_{x,uv\ldots}{}^{is} \rangle = \langle R_{x,yuv\ldots}{}^{is} \rangle + \langle R_{x,\bar{1}uv\ldots}{}^{is} \rangle \langle R_{1,y}' \rangle = \langle R_{x,\bar{1}uv\ldots}{}^{is} \rangle \langle R_{1,y} \rangle, \quad (36)$$

where we use

$$\langle R_{x,y} \rangle = \Delta_{\mathrm{Ret}}'(x-y) + \langle R_{x,y}' \rangle, \quad (37)$$

which follows from (30) and is depicted in Fig. 2, a

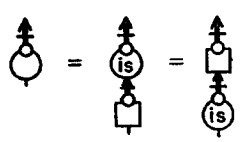

FIG. 3. Analysis of $\langle R_{x,y}' \rangle$, Eqs. (39) and (41).

square denoting the amputated unprimed functional. Thus, we find from (32)

$$\langle R_x' \rangle = \langle R_x{}^{is} \rangle \quad (38)$$

and with (36)

$$\langle R_{x,u}' \rangle = \langle R_{x,u}{}^{is} \rangle + \langle R_{x,\bar{1}}{}^{is} \rangle \langle R_{1,u}' \rangle = \langle R_{x,\bar{1}}{}^{is} \rangle \langle R_{1,u} \rangle, \quad (39)$$

$$\langle R_{x,uv}' \rangle = \langle R_{x,uv} \rangle = \langle R_{x,\bar{1}\bar{2}}{}^{is} \rangle \langle R_{1,u} \rangle \langle R_{2,v} \rangle + \langle R_{x,\bar{1}}{}^{is} \rangle \langle R_{1,uv} \rangle, \quad (40)$$

etc. The iteration of (39)

$$\langle R_{x,u}' \rangle = \langle R_{x,u}{}^{is} \rangle + \sum_{n=1}^{\infty} \langle R_{x,\bar{1}}{}^{is} \rangle \langle R_{1,\bar{2}}{}^{is} \rangle \cdots \langle R_{n,u}{}^{is} \rangle$$

can be resummed to give

$$\langle R_{x,u}' \rangle = \langle R_{x,u}{}^{is} \rangle + \langle R_{x,\bar{1}}' \rangle \langle R_{1,u}{}^{is} \rangle = \langle R_{x,\bar{1}} \rangle \langle R_{1,u}{}^{is} \rangle, \quad (41)$$

which proves (41) since the sum breaks off in any finite order of J. Multiplication of (40) by $\langle R_{y,\bar{z}} \rangle$ and use of (41), (37) give

$$\langle R_{x,uv} \rangle = \langle R_{x,\bar{y}} \rangle \langle R_{y,\bar{1}\bar{2}}{}^{is} \rangle \langle R_{1,u} \rangle \langle R_{2,v} \rangle. \quad (42)$$

Equations (39) and (41), and (40) and (42) are depicted in Figs. 3 and 4. Though these figures closely resemble those of ordinary graphs, they actually show "meta-graphs," because by functional differentiation and use

of (36) an arbitrary number of additional external lines[27] can be attached to them.

Let us insert (14) into (18). This gives

$$:\exp\left[\int duA_{\text{in}}(u)\mathbf{K}_u\delta/\delta J(u)\right]:(\langle R_{x,y}\rangle-\langle R_{y,x}\rangle)$$

$$=:\exp\left[\int duA_{\text{in}}(u)\mathbf{K}_u\delta/\delta J(u)\right]:$$

$$\cdot\left\{\exp\left[\int\int du'du''\frac{\delta}{\delta J'(u')}\mathbf{K}_{u'}i\Delta^+(u'-u'')\right.\right.$$

$$\left.\times\mathbf{K}_{u''}\frac{\delta}{\delta J''(u'')}\right]-\exp\left[\int\int du'du''\frac{\delta}{\delta J'(u')}\right.$$

$$\left.\left.\times\mathbf{K}_{u'}i\Delta^+(u''-u')\mathbf{K}_{u''}\frac{\delta}{\delta J''(u'')}\right]\right\}$$

$$\cdot i\langle R_x\{J+J'\}\rangle\langle R_y\{J+J''\}\rangle\,|_{J'=J''=0}. \quad (43)$$

What counts for the "structure" of the right-hand side is not which intermediate states did contribute in (18),

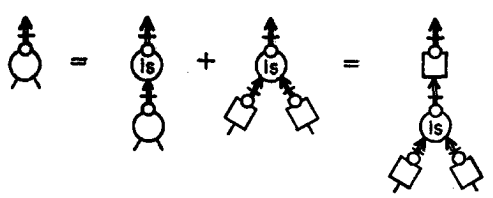

FIG. 4. Analysis of $\langle R_{x,uv'}\rangle$, Eq. (40).

but how many contraction lines connect the two factor functionals, which are connected within themselves. It is one connecting line, then a $i\Delta$-line, which in general gives rise to several separate one-particle singularities (singularities on mass hyperboloids) in momentum space, their position depending on where the external particles, represented by $\int du f_\alpha \mathbf{K}_u\delta/\delta J(u)$, are attached, rather than a one-particle intermediate state; this latter being the case only for the vacuum expectation value of (43) with $J=0$. In addition, there will be the singularities studied before of the factors in (43) of the retarded or advanced type, respectively, lying in momentum space on the same hyperboloids[28] as the intermediate states singularities just described. Since both sides of (43) are equal, these singularities must altogether cancel leaving a remainder that is finite in the first place and must be shown to vanish in the next step; this means, is open for the many-particle structure analysis of later sections.

Clearly, in order to satisfy (43) it is sufficient to do so for the vacuum expectation value,

$$\langle R_{x,y}\rangle-\langle R_{y,x}\rangle=i\langle[R_x,R_y]\rangle. \quad (44)$$

From (37) and (14) we find

$$R_x=A_{\text{in}}(x)+\int dx_1\Delta_{\text{Ret}}'(x-x_1)J(x_1)+R_x'.$$

Upon use of (13), (44) takes the form[29]

$$\langle R_{x,\bar u}'\rangle\Delta_{\text{Ret}}''(y-u)-\Delta_{\text{Ret}}''(x-u)\langle R_{y,\bar u}'\rangle$$
$$-\Delta''(x-y)=i\langle[R_x',R_y']\rangle, \quad (45)$$

where the abbreviations

$$\Delta_{\text{Ret}}''\equiv\Delta_{\text{av}}'-\Delta,\quad \Delta''\equiv\Delta'-\Delta$$

have been used. With (39) we rewrite (45) as follows:

$$\langle R_{x,\bar u^{is}}\rangle\Delta_{\text{Ret}}''(y-u)+\langle R_{x,\bar 1^{is}}\rangle\langle R_{1,\bar u}'\rangle\Delta_{\text{Ret}}''(y-u)$$
$$-\Delta_{\text{Ret}}''(x-u)\langle R_{y,\bar u^{is}}\rangle-\Delta_{\text{Ret}}''(x-u)\langle R_{2,\bar u}'\rangle\langle R_{y,\bar 2^{is}}\rangle$$
$$-\Delta''(x-y)=i\langle[R_x',R_y']\rangle=i\langle[R_x',R_y']^i\rangle$$
$$+i\langle R_{x,\bar 1^{is}}\rangle\langle[R_1',R_y']\rangle+i\langle[R_x',R_1']\rangle\langle R_{y,\bar 1^{is}}\rangle$$
$$-i\langle R_{x,\bar 1^{is}}\rangle\langle[R_1',R_2']\rangle\langle R_{y,\bar 2^{is}}\rangle$$
$$-\langle R_{x,\bar u^{is}}\rangle\Delta(u-v)\langle R_{y,\bar v^{is}}\rangle. \quad (46)$$

Here the second equality sign defines $i\langle[R_x',R_y']^i\rangle$. The terms subtracted out denote in order: all one-particle singularities from $\langle R_x\rangle$, all one-particle singularities from $\langle R_y\rangle$, correction for twice-subtracted terms, one-particle intermediate state singularity not yet taken into account.

Note that all subtractions, except the last one, also contain contributions that are not singular, because Δ_{Ret}', that makes up bridges, has also a nonsingular part whose treatment is a matter of convention. In addition, often at the place where Δ_{Ret}' is singular, the subtracted term vanishes because of momentum conservation.

The definition of one-particle singularities (or reducibilities) used here, which is suggested by perturbation theory, turns out to be the most convenient one, as we shall repeatedly see.

We now replace on the right-hand side of (46) everywhere $i\langle[R_1',R_y']\rangle$ etc., by their values given by (45). Thereupon, with (39), all one-particle reducibilities drop out, and (46) reduces to

$$\langle R_{x,\bar u^{is}}\rangle\Delta_{\text{Ret}}'(y-u)-\Delta_{\text{Ret}}'(x-u)\langle R_{y,\bar u^{is}}\rangle$$
$$-\Delta''(x-y)=i\langle[R_x',R_y']^i\rangle. \quad (47)$$

It is convenient to amputate the Δ_{Ret}'-functions at x and y to obtain the simple equation[30]

$$\langle R_{\bar x,\bar y^{is}}\rangle-\langle R_{\bar y,\bar x^{is}}\rangle-\Delta''(\bar x-\bar y)=i\langle[R_{\bar x}',R_{\bar y}']^i\rangle, \quad (48)$$

[27] Because of this capacity, "metagraphs" represent not only the vacuum expectation value, but, with (14), all matrix elements of an operator product. Note that since $\langle R_{x,y'}\rangle|_{J=0}=\langle R_{x,y^i}\rangle|_{J=0}=\langle R_{x,y^{is}}\rangle|_{J=0}=0$, Fig. 3 becomes a triviality in lowest order of J.

[28] Of course, they may occasionally be ruled out because of energy-momentum conservation.

[29] Note that on the mass shell Δ_{Ret}'-amputation is equivalent to application of the Klein-Gordon operator.

[30] Equation (48) is equivalent to (44) since all one-particle reducibilities can be correctly recovered, as is shown by comparing (44) and (48) in ascending powers of J. See, however, note added in proof.

whose zero-order part in J

$$-\Delta''(\bar{x}-\bar{y})=i\langle[R_{\bar{x}}',R_{\bar{y}}']^{i}\rangle|_{J=0} \tag{49}$$

will be studied in Sec. 5.

Equation (48) shows that the absorptive part of $\langle R_{\bar{x},\bar{y}}{}^{is}\rangle$ has no one-particle intermediate-state contribution. It also has, as a consequence of (48) and the retardedness condition (12), no retarded or advanced one-particle singularity. Unfortunately, we can prove this here only by going back to the full functional $\langle R_x\rangle$. Equation (48), together with (12) and (30), (38) etc., yields a local field for which the proof given at the beginning of this section is applicable. Thus, the one-particle singularities of $\langle R_x\rangle$ are known, and since they have been subtracted out as described after (46), (48) does not contain them any more. Presumably, a more direct proof on the basis of (48), (12) is possible.

Equation (48) can be given a different form by expanding the right-hand side as in (43), using (39), (40) etc., to express everything in terms of $\langle R^{is}\rangle$. With the abbreviation,

$$\begin{aligned} i\Delta^{+s}(x-y)\equiv \sum_{m,n=0}^{\infty} &\langle R_{x,\bar{1}}{}^{is}\rangle\langle R_{1,\bar{2}}{}^{is}\rangle\cdots \\ &\times\langle R_{m-1,\bar{m}}{}^{is}\rangle i\Delta^{+}(x_m-y_n) \\ &\cdot\langle R_{(n-1)',\bar{n}'}{}^{is}\rangle\cdots\langle R_{\bar{1}',2'}{}^{is}\rangle\langle R_{y,\bar{1}'}{}^{is}\rangle, \end{aligned} \tag{50}$$

we obtain[31]

$$\begin{aligned} &\langle[R_{\bar{x}}',R_{\bar{y}}']^{i}\rangle \\ &=\sum_{n=2}^{\infty}\frac{1}{n!}\langle R_{\bar{x},\bar{1}\bar{2}\cdots\bar{n}}{}^{is}\rangle i\Delta^{+s}(1,1')\cdots i\Delta^{+s}(n,n') \\ &\quad\cdot\langle R_{\bar{y},\bar{1}'\bar{2}'\cdots\bar{n}'}{}^{is}\rangle+\sum_{n=4}^{\infty}\frac{1}{(n-2)!}\langle R_{\bar{x},\bar{1}\bar{2}}{}^{is}\rangle \\ &\quad\times\langle R_{2,\bar{3}\bar{4}\cdots\bar{n}}{}^{is}\rangle i\Delta^{+s}(1,1')i\Delta^{+s}(3,3') \\ &\quad\cdot i\Delta^{+s}(4,4')\cdots i\Delta^{+s}(n,n')\langle R_{\bar{y},\bar{1}'\bar{3}'\cdots\bar{n}'}{}^{is}\rangle+\cdots, \end{aligned} \tag{51}$$

where further formal tools could be introduced. We only remark that if (51) is used in (48), it is readily seen from the exponential structure of (35) that all s signs in (48), (50), and (51) can simultaneously be dropped,[32] as one would have expected.

The question of whether in (48) the functional $\langle R_{\bar{x},\bar{y}}{}^{is}\rangle$ can be singled out by multiplication of both sides with $\theta(x-y)$ will be discussed in Sec. 5.

We have seen that (44) can be formulated entirely in terms of one-particle irreducible functionals, the one-particle singularities cancelling. We plan to eliminate in the next step the two-particle singularities in (48) and to express it in terms of two-particle irreducible functionals. We found it too difficult to perform this next step in the same generality as the first one, because the various possibilities of two-particle cuts in a general graph are complicated to disentangle. We shall be more modest and will first present for purposes of illustration the method to be used in the next section here, in application to the much simpler one-particle case.

Let us restrict our attention to the one-particle reducibilities of the functional $\langle R_{x,yz\cdots}\rangle$ between x and the whole group $yz\cdots$. The ansatz,

$$\langle R_{x,yz\cdots}{}'\rangle=\langle R_{x,1}\rangle\langle\tilde{R}_{\bar{1},yz\cdots}{}^{i}\rangle \tag{52}$$

defines a functional $\langle\tilde{R}_{1,yz\cdots}{}^{i}\rangle$ because with (39) and (37) it can be solved to give

$$\langle\tilde{R}_{x,yz\cdots}{}^{i}\rangle=\langle R_{x,yz\cdots}{}'\rangle-\langle R_{x,\bar{1}}{}^{is}\rangle\langle R_{1,yz\cdots}{}'\rangle.$$

The indices of $\langle\tilde{R}_{x,yz\cdots}{}^{i}\rangle$ do not denote functional derivatives.

We rewrite (52) as

$$R_x'=r(x,1)\tilde{R}_{\bar{1}}{}^{i}, \tag{53}$$

which is to express that if R_x' is inserted into a commutator or anticommutator and, if as in (43) contraction differentiations are to be carried out, $r(x,1)$, though being numerically equal to $\langle R_{x,1}\rangle$, must not be differentiated, but (52) should be used instead. With (37), (39) we can rewrite (53) as

$$R_x'=\tilde{R}_x{}^{i}+r_i(x,\bar{1})R_1', \tag{54}$$

where $r_i(x,\bar{1})$ numerically equals $\langle R_{x,\bar{1}}{}^{is}\rangle$ but must, as before $r(x,1)$, not be differentiated for contractions. It is convenient to rewrite (54) as

$$R_x'=\tilde{R}_x{}^{i}+r_i(x,\bar{1})R_1, \tag{55}$$

where

$$\tilde{R}_x=\begin{cases}0 \text{ if once differentiated}\\ \tilde{R}_x{}^{i} \text{ if at least twice differentiated}\end{cases} \tag{56}$$

for purposes of contraction. We depict (53) and (54) in Fig. 5. The broken lines indicate where contraction differentiations should be applied. Other differentiations

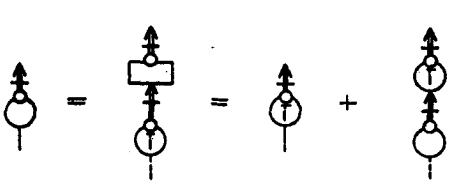

FIG. 5. Alternative analysis of $\langle R_x'\rangle$, Eqs. (53) and (54).

[31] Here infinite sums seem to occur, but because of $\langle R_{x,y}{}^{is}\rangle|_{J=0}=0$ in each finite order of J only a finite number of terms in (50) and (51) do not vanish. An infinite number of intermediate particles, however, means that also external relative momenta must be infinite because of frequency conditions.

[32] Equation (35) shows that the s sign can be replaced by operating with an exponential functional differential operator on both sides of (48). By considering ascending powers of J, one shows by complete induction that the exponential operator could have been omitted because of $\langle R_1'\rangle|_{J=0}=\langle R_{1,y}'\rangle|_{J=0}=0$.—We could have obtained this result more easily by introducing, following J. Schwinger, footnote 18, $\hat{J}(x)$ instead of $J(x)$ as variable, see (34). For other purposes, however, this change does not prove convenient.

can be carried out either like contraction differentiations or as general differentiations of all functionals.[33]

We now insert (53) and (54) into (44) in the following way: in all terms we shall exhibit the one-particle reducibility between x and y nearest to x, if there is any. With (37), the equation after (44), and (13) this gives[29]

$$\begin{aligned} r_i(x,\bar{u})\langle R_{u,y}\rangle &+\Delta_{\mathrm{Ret}}'(x-y) \\ &+\langle \bar{R}_{x,y^i}\rangle-\langle \bar{R}_{\bar{u},x^i}\rangle r(y,u)-\Delta_{\mathrm{Ret}}'(y-x) \\ =&-\Delta(x-u)\langle R_{y,\bar{u}}\rangle+r_i(x,\bar{u})i\langle[R_u,R_y]\rangle \\ &-\langle \bar{R}_{x,\bar{u}^i}\rangle\Delta(u-y)+i\langle[\bar{R}_{x^i},\bar{R}_{\bar{u}^i}]\rangle r(y,u). \quad (57) \end{aligned}$$

In analogy to (45) we write

$$i\langle[\bar{R}_{\bar{x}^i},R_{\bar{u}^i}]\rangle=r_i(\bar{x},\bar{u})-r_i(\bar{u},\bar{x})-\Delta''(\bar{x}-\bar{u})-\psi(\bar{x},\bar{u}), \quad (58)$$

which defines the functional $\psi(\bar{x},\bar{u})$. Upon use of (58), (44), (56), and (53) in (57) we obtain

$$\Delta_{\mathrm{Ret}}'(x-u)\psi(\bar{u},\bar{v})r(y,v)=0, \quad (59)$$

wherefrom $\psi(\bar{u},\bar{v})=0$ follows.[34] Thus (58) becomes, because of (56), identical with (48).

A third method, and actually the simplest one, is to insert (53) into (45). However, this method is not practical in the two-particle case.

Insertion of (53) and (55) into (19) etc., allows to exhibit, for instance, in the manner explained before (57), the one-particle reducibilities. However, we shall not need the formulas obtained, which in all cases can also be written down by inspection.

The Eqs. (44) or (47) also give one-particle singularities from the Δ_{Ret}-parts of the end lines leading to x or y, according to (15), (16). Equating the residua on both sides of those equations gives the unitarity condition. This technique is analogous to Zimmermann's for deriving the asymptotic condition.[23] Of course, here the interchangebility of integrations has been assumed, by reference to Zimmermann's work.[10]

As a useful result of this section we shall keep in mind that one-particle singularities always cancel when (44) or (45) are used and can be dropped at an arbitrary stage of the calculation.

3. TWO-PARTICLE STRUCTURE

Type of Singularities

Retarded functions have singularities as a consequence of two-particle cuts in double graphs. These singularities are analogous to those Feynman amplitudes have as a consequence of two-particle cuts in Feynman graphs and appear at the threshold of a real two-particle energy, which is $2m$ in our case. The character of these singularities is derivable from unitarity and the relevant two-particle phase space factor.

In a double graph there are, as (25) shows, several types of two-particle cuts. One may cut two Δ_{Ret}-lines, one Δ_{Ret}- and one Δ_{Av}-line, and one Δ_{Ret}- and one $\Delta_1/2$-line. Let us discuss the integrals,

$$\begin{aligned} &H_{R,A,1}(x\cdots,y\cdots) \\ &=\int\int dzdz'dudu'F(x\cdots,zz') \\ &\qquad\times\Delta_{\mathrm{Ret}}(z-u)\Delta_{\mathrm{Ret,Av},1}(z'-u')G(y\cdots,uu'). \end{aligned}$$

For the singularity under consideration, the functions F and G merely act as short-range form factors, which provide a cutoff for the otherwise divergent integrals obtained by replacing F and G by point functions. If p is the momentum conjugate to $x-y$, and thus the momentum transported by the two cut lines, with $z=p^2-4m^2$ one finds for the Fourier transforms of H_R and H_1 a singularity of the type const $(-z)^{\frac{1}{2}}$, where for $z>0$ the branch is to be chosen according to the sign of p_0, and no singularity for H_A. Nevertheless, this last type of cut has to be taken into account since otherwise the elimination of the two-particle intermediate states in the absorptive parts of the "irreducible" functions would not be possible. In (44) the singularities just considered of the left-hand side will be equalled on the right-hand side if it is written as in (43) by similar two-particle singularities in the two factors of the retarded and advanced type, respectively, and by terms with a two-particle intermediate state where the pairs of lines $i\Delta^+\cdot i\Delta^+$ and $(-i\Delta^-)\cdot(-i\Delta^-)$ give the singularities const$\theta(z)\theta(p_0)(z)^{\frac{1}{2}}$ and const$\theta(z)\theta(-p_0)(z)^{\frac{1}{2}}$, respectively.

Choice of Equations

If we follow the method explained in the last section, we have to choose an ansatz that is the analog of (53) and (55), or Fig. 5. The enumeration of possible two-particle cuts just given, as well as inspection of (25) to determine the factors[35] leads to

$$R_{x,\,yzu}=\frac{1}{2}r(x,y12)R_{\bar{1}\bar{2},zu^i}+r(x1,y2)R_{\bar{2},\bar{1}zu^i} \quad (60)$$

as the analog of (53), where numerically

$$r(x,y12)=\langle R_{x,y12}\rangle, \quad r(x1,y2)=\langle R_{x1,y2}\rangle.$$

In this section barring of coordinates is to indicate the absence of the full one-particle reducible parts (cf., Fig. 4), and not of Δ_{Ret}' or Δ_{Av}' alone.[36] Equation (60) is

[33] Of course, "contraction differentiations" are ordinary functional differentiations, but we find it convenient for our purposes to deal with them as explained.

[34] Multiply (59) from the right by $r_i(v,w)$, integrate and use (41), (37), and again (59). See, however, note added in proof.

[35] For instance, the factor of the last term of the right-hand side of (60), i.e., with a retarded and an advanced line, is obtained by functionally differentiating (25) with respect to $\bar{J}$ and J. The Δ_1-part from the first differentiation does not contribute since there must be at least one retarded line on the cut.

[36] Barring, always applied to the irreducible functionals, can be made part of their definition such that nonbarring of z means multiplication of $R_{\bar{1}\bar{2},\bar{3}u^i}$ by $\langle R_{3,z}\rangle$ and integrating over 3. Note that the irreducible functionals are always connected. They do not contain terms of the form $\langle R_{1,3}\rangle K_3\Delta_1(3-4)\cdot R_{\bar{2},\bar{4}zu^i}$.

depicted in Fig. 6, where a simple line stands for the function $\Delta_1/2$ and the stroke indicates where contraction differentiations (besides z and u) are to be applied. The graph with the $\Delta_1/2$-line is absorbed in the first term on the right-hand side of (60) because $r(x1,y2)$ according to (19) also contains

$$\frac{1}{2}\langle\{R_x,A_{\text{in}}(1)\}_{y2}\rangle=\frac{1}{2}\langle\{R_{x,y2},A_{\text{in}}(1)\}\rangle,$$

which can be evaluated with (17) to give just the required term. The functionals $R_{\bar{1}\bar{2},zu}{}^i$ and $R_{\bar{2},\bar{1}zu}{}^i$ are two-irreducible between 1, 2 and z, u in an intuitive sense to be made precise later.

Since two R^i functionals appear in (60), it has to be supplemented by the ansatz

$$R_{xy,zu}{}'=\frac{1}{2}r(xy,12)R_{\bar{1}\bar{2},zu}{}^i+r(xy1,2)R_{\bar{2},\bar{1}zu}{}^i, \quad (61)$$

where

$$\langle R_{xy,zu}{}'\rangle=\langle R_{xy,zu}\rangle-\langle R_{x,z}\rangle\langle R_{y,u}\rangle-\langle R_{x,u}\rangle\langle R_{y,z}\rangle \quad (62)$$

in analogy to (37). The use of this definition of the primed functional is convenient here because it allows $R_{\bar{1}\bar{2},zu}{}^i$ to be connected.

In order to obtain complete analogy to the system (53), (55) we have to introduce two more equations of the type (53), namely

$$R_{xz,yu}{}'=\frac{1}{2}r(x,y12)R_{\bar{1}\bar{2}z,u}{}^i+r(x1,y2)R_{\bar{2}z,\bar{1}u}{}^i, \quad (z_0<u_0) \quad (63)$$

and

$$R_{xyz,u}{}'=\frac{1}{2}r(xy,12)R_{\bar{1}\bar{2}z,u}{}^i+r(xy1,2)R_{\bar{2}z,\bar{1}u}{}^i, \quad (z_0<u_0), \quad (64)$$

where the time restriction is necessary since otherwise an additional term with two advanced lines would have been needed, and the prime of $R_{xyz,u}{}'$ denotes the connected part similar to (62).

The vacuum expectation values of (60), (61), (63), and (64) together can be written in the symbolic form

$$'F'=('1+'F')F_i'. \quad (65)$$

Here $'F'$ is the two-by-two matrix with the elements

$$'F'_{11}=\frac{1}{2}r'(xy,zu), \quad 'F'_{12}=\frac{1}{\sqrt{2}}r'(xyu,z),$$
$$'F'_{21}=\frac{1}{\sqrt{2}}r(x,yzu), \quad 'F_{22}{}'=r'(xu,yz), \quad (66)$$

where $r'(xy,zu)$ is defined as in (62) and similarly $r'(xyu,z)$ and $r'(xu,yz)$. $'F'_i$ is the same matrix with the irreducible functionals, and absence of a prime means removal of one-particle reducibilities. $1'='1$ is the unamputated "unit matrix" with the elements

$$'1_{11}=\frac{1}{2}r(x,z)r(y,u)+\frac{1}{2}r(x,u)r(y,z),$$
$$'1_{12}=\frac{1}{\sqrt{2}}r(x,z)r(yu)+\frac{1}{\sqrt{2}}r(xu)r(y,z),$$
$$'1_{21}=0,$$
$$'1_{22}=r(x,z)r(u,y),$$

and matrix multiplication implies integration over the interior coordinates.

We now write down, according to the symbolic equation

$$'F'='F_i('1+'F'), \quad (67)$$

the four equations analogous to (55), namely[36,37]

$$R_{x,yzu}=\tilde{R}_{x,yzu}{}^i+\frac{1}{2}r_i(x,y\bar{1}\bar{2})R_{12,zu}+r_i(x\bar{1},y\bar{2})R_{2,1zu}, \quad (68)$$

$$R_{xy,zu}{}'=\tilde{R}_{xy,zu}{}^i+\frac{1}{2}r_i(xy,\bar{1}\bar{2})R_{12,zu}+r_i(xy\bar{1},\bar{2})R_{2,1zu}, \quad (69)$$

$$R_{xz,yu}{}'=\tilde{R}_{xz,yu}{}^i+\frac{1}{2}r_i(x,y\bar{1}\bar{2})R_{12z,u}+r_i(x\bar{1},y\bar{2})R_{2z,1u}, \quad (z_0<u_0), \quad (70)$$

and

$$R_{xyz,u}{}'=\tilde{R}_{xyz,u}{}^i+\frac{1}{2}r_i(xy,\bar{1}\bar{2})R_{12z,u}+r_i(xy\bar{1},\bar{2})R_{2z,1u}, \quad (z_0<u_0), \quad (71)$$

where, in analogy to (56),[38]

$$\langle\tilde{R}_{x,yzu}{}^i\rangle=\langle R_{x,yzu}{}^i\rangle-\frac{1}{2}r_i(x,y\bar{1}\bar{2})(\langle R_1\rangle\langle R_2\rangle)_{zu} \quad (72)$$

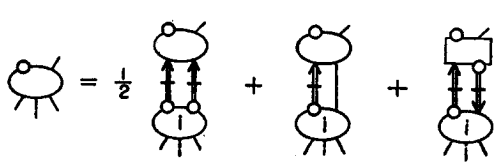

FIG. 6. Two-particle structure of $\langle R_{x,yzu}\rangle$, Eq. (60).

[37] By integration of the field equation in the Heisenberg representation, G. Källén, CERN/T/GK-2, obtained some of the equations mentioned in footnote 18a and found the ladder approximation of (69) as Bethe-Salpeter equation.

[38] This is seen if (56) is replaced by the explicit definition $\tilde{R}_x{}^i=R_x{}^i-\int d1 r_i(x,1)J(1)$ where for contractions only J but not $r_i(x,1)$ is to be differentiated. Similarly, the notation of (72) is meant, where for contractions only $\langle R_1\rangle$ and $\langle R_2\rangle$ but not $r_i(x,y\bar{1}\bar{2})$ are to be differentiated. Equation (72) is only correct up to one-particle reducible parts which, however, are always dropped.

and similarly for the other $\tilde{R}^i$. Equation (68) is depicted in Fig. 7.

Discussion of Equations (65), (67)

The vacuum expectation values of (60), (61) can be taken as determining equations for $r_i(\bar{1}\bar{2},zu)$ and $r_i(\bar{2},\bar{1}zu)$, and (63), (64) for $r_i(\bar{1}\bar{2}z,u)$, $(z_0<u_0)$, and $r_i(\bar{2}z,\bar{1}u)$, $(z_0<u_0)$. On the other hand, (68), (70) could be chosen for $r_i(x,y\bar{1}\bar{2})$ and $r_i(x\bar{1},y\bar{2})$, $(1_0<2_0)$, and (69), (71) for $r_i(xy,\bar{1}\bar{2})$ and $r_i(xy\bar{1},\bar{2})$, $(1_0<2_0)$. Since the iterative solutions of those pairs of equations do not break off, contrary to the situation in the last section, a more general discussion is here required.

For (65) to have a solution F_i', there must not be a left eigenvector of $(1'+'F')$ to the eigenvalue zero. The solution is unique if there is also no such right eigenvector. For (67) right and left are interchanged. From

$$(1'+'F')(1-F_i')=(1-'F_i)(1'+'F')=1' \quad (73)$$

it easily follows that if both Eqs. (65) and (67) should have solutions, both F_i are unique and equal. This is the only situation we are interested in. Since from (73) we derive[39]

$$\frac{\delta}{\delta J}F_i'=(1-F_i')\cdot\frac{\delta}{\delta J}F'\cdot(1-F_i'), \quad (74)$$

it suffices to consider (73) in lowest (zero) order of J, all higher orders of F_i' being obtainable with the help of (74) from lower orders. In zero order of J (73) reduces to a relativistically invariant integral relation between four-point functions. Because of translational invariance, we take the Fourier transforms of (73) with respect to the distance between the later coordinate of the later pair x, y and the later coordinate of the earlier pair z, u, in a fixed coordinate system. Since this distance has nonnegative time component, the Fourier transforms $\tilde{F}(K,\Delta,\Delta')$ and $\tilde{F}_i(K,\Delta,\Delta')$, where Δ and Δ' are the relative coordinates of the later and the earlier pair, are analytic in the upper K_0 half plane. $\tilde{F}(K,\Delta,\Delta')$ will not be one-particle singular at some discrete real K since we assume that all these reducibilities in the equations have been removed.[40]

We now have to assume that (73), in zero order of J, possesses a solution of the form

$$\tilde{F}_i(K,\Delta,\Delta')=\tilde{F}(K,\Delta,\Delta')+\int\tilde{F}(K,\Delta,\Delta'')\tilde{R}(K,\Delta'',\Delta')d\Delta'', \quad (75)$$

where the resolvent $\tilde{R}(K,\Delta,\Delta')$ is analytic in the upper K_0 half plane up to discrete singularities, at which we

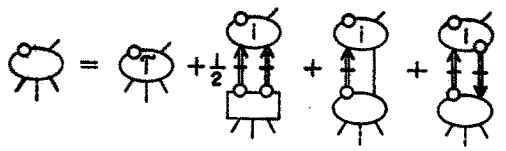

FIG. 7. Alternative analysis of $\langle R_{x,yzu}\rangle$, Eq. (68).

choose in (75) the retarded boundary condition.[41] We hope that a more intensive study of (73), using properties of retarded four-point functions, will lead to such, or an equivalent, result and expect the analyticity property of $F(K,\Delta,\Delta')$ in the K_0 half plane to be important in this connection.

The $r_i(x,y\bar{z}\bar{u})$ etc., being determined, the higher contraction derivatives $R_{x,y\bar{z}\bar{u}v}{}^i$ etc., can be found from (74), and with (73) easily shown to solve (60), (61), (63), and (64).

Result of Substitution in (44)

Equations (68) and (60) are now inserted into (44) in the same manner as (55) and (53) were. The calculation is given in the appendix, and we state the result.

Define, in analogy to (58), three functionals $X^i(\bar{x}\bar{1}\bar{2},\bar{y})$, $Y^i(\bar{x}\bar{1},\bar{2}\bar{y})$, and $Z^i(\bar{x}\bar{1},\bar{2}\bar{y})$ by the equations

$$\begin{aligned}X^i(\bar{x}\bar{1}\bar{2},\bar{y})=&r_i(\bar{1}\bar{2},\bar{x}\bar{y})-r_i(\bar{1}\bar{x},\bar{2}\bar{y})-r_i(\bar{2}\bar{x},\bar{1}\bar{y})\\&+\tfrac{1}{2}\langle\{\tilde{R}_{\bar{1},\bar{2}\bar{y}}{}^i,R_{\bar{x}}\}^i\rangle+\tfrac{1}{2}\langle\{\tilde{R}_{\bar{1},\bar{z}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i\}^i\rangle\\&+\tfrac{1}{2}\langle\{\tilde{R}_{\bar{2},\bar{1}\bar{y}}{}^i,R_{\bar{x}}\}^i\rangle+\tfrac{1}{2}\langle\{\tilde{R}_{\bar{2},\bar{1}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i\}^i\rangle\\&-i\langle[\tilde{R}_{\bar{1}\bar{2}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i]^i\rangle-i\langle[\tilde{R}_{\bar{1}\bar{2},\bar{y}}{}^i,R_{\bar{x}}]^i\rangle\\&-i\langle[(R_{\bar{1}}R_{\bar{2}}),\tilde{R}_{\bar{x},\bar{y}}{}^i]^i\rangle-i\langle[(R_{\bar{1}}R_{\bar{2}})_{\bar{y}},R_{\bar{x}}]^i\rangle, \quad (76)\end{aligned}$$

$$\begin{aligned}Y^i(\bar{1}\bar{x},\bar{2}\bar{y})=&r_i(\bar{1},\bar{x}\bar{2}\bar{y})-r_i(\bar{x},\bar{1}\bar{2}\bar{y})\\&-i\langle[R_{\bar{1},\bar{y}},R_{\bar{x},\bar{2}}]^i\rangle-i\langle[R_{\bar{1}},\tilde{R}_{\bar{x},\bar{y}\bar{2}}{}^i]^i\rangle\\&-i\langle[\tilde{R}_{\bar{1},\bar{2}\bar{y}}{}^i,R_{\bar{x}}]^i\rangle-i\langle[\tilde{R}_{\bar{1},\bar{2}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i]^i\rangle, \quad (77)\end{aligned}$$

$$\begin{aligned}Z^i(\bar{1}\bar{x},\bar{2}\bar{y})=&r_i(\bar{1}\bar{x},\bar{2}\bar{y})-\tfrac{1}{2}\langle\{R_{\bar{1},\bar{y}},R_{\bar{x},\bar{2}}\}^i\rangle\\&-\tfrac{1}{2}\langle\{R_{\bar{1}},\tilde{R}_{\bar{x},\bar{y}\bar{2}}{}^i\}^i\rangle-\tfrac{1}{2}\langle\{\tilde{R}_{\bar{1},\bar{2}\bar{y}}{}^i,R_{\bar{x}}\}^i\rangle\\&-\tfrac{1}{2}\langle\{\tilde{R}_{\bar{1},\bar{z}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i\}^i\rangle, \quad (78)\end{aligned}$$

[39] Note that primes can be removed by the procedure explained in footnote 34.

[40] Therefore, the homogeneous Bethe-Salpeter equation $(1-'F_i)A=0$ no longer has a solution.

[41] This is meant as follows: the equation $f(K_0)(K_0-C)=1$ has no solution for $K_0=C$, but for the K_0-integration to be performed afterwards we use the solution $f(K_0)=(K_0+i\epsilon-C)^{-1}$, $\epsilon\to 0$. Singularities at $\mathrm{Im}K_0>0$ require a contour deformation. Since a function that vanishes on an interval and is analytic in the half plane vanishes identically, we expect only discrete singularities of $R(K,\Delta,\Delta')$, which can be tackled as described. Note also that due to (75) the property $r(x,yzu)=0$ unless y is timelike advanced with respect to x implies the same property for $r_i(x,yzu)$.

which correspond to the equations[42]

$$i[R_{12},R_x]_y=R_{12,xy}-R_{1x,2y}-R_{2x,1y}+\frac{1}{2}\{R_{1,2},R_x\}_y+\frac{1}{2}\{R_{2,1},R_x\}_y, \quad (79)$$

(18), and (19), respectively. These functionals satisfy the linear homogeneous equation

$$\frac{1}{2}X^i(\bar{x}\bar{1}\bar{2},\bar{y})r(z,u12)+\frac{1}{2}Y^i(\bar{1}\bar{x},\bar{2}\bar{y})\langle\{R_{z,1},R_2\}_u\rangle+iZ^i(\bar{1}\bar{x},\bar{2}\bar{y})\langle[R_{z,1},R_2]_u\rangle=0, \quad (80)$$

which is the analog of (59).

The meaning of the brackets $\{\ \}^i$ and $[\ ]^i$, denoting the two-particle irreducible part of the anticommutator or commutator, will be explained later.

Another linear homogeneous relation between X^i, Y^i, and Z^i is obtained from (20), written as

$$R_{zu,xy}=\frac{1}{2}\{R_{x,u},R_z\}_y+\frac{1}{2}\{R_{x,z},R_u\}_y-i[R_x,R_{zu}]_y$$

by using (61) and (68). The method of the appendix gives

$$\frac{1}{2}X^i(\bar{x}\bar{1}\bar{2},\bar{y})r(zu,12)-\frac{i}{4}Y^i(\bar{1}\bar{x},\bar{2}\bar{y})\{\langle[R_{2,u},R_{z,1}]\rangle+\langle[R_{2,z},R_{u,1}]\rangle\}-\frac{1}{4}Z^i(\bar{1}\bar{x},\bar{2}\bar{y})[\langle\{R_{2,u},R_{z,1}\}\rangle+\langle\{R_{2,z},R_{u,1}\}\rangle-2i\langle[R_2,R_{zu,1}]\rangle]=0, \quad (81)$$

which is the analog of an equation for one-particle reducibilities we did not give.

A relation between Y^i and Z^i alone is obtained from

$$R_{xz,yu}=\frac{1}{2}\{R_z,R_z\}_{yu},$$

derived from (19), upon use of (70), (68), and (60). It is

$$\frac{i}{4}Y^i(\bar{x}\bar{1},\bar{2}\bar{y})\langle[R_{z,1},R_{2,u}]\rangle+\frac{1}{2}Z^i(\bar{1}\bar{x},\bar{2}\bar{y})\langle\{R_{z,1},R_{2,u}\}\rangle=0, \quad (z_0<u_0). \quad (82)$$

The time restriction implies $1_0<2_0$.

If in the last example the restriction $z_0<u_0$ is dropped, it is necessary to add in (70) the fourth term $\frac{1}{2}r_i(x\bar{1}\bar{2},y)R_{z,u12}$. Thereupon one obtains instead of (82), the equation

$$\frac{i}{4}Y^i(\bar{1}\bar{x},\bar{2}\bar{y})[-ir(z,u12)+\langle[R_{z,1},R_2]_u\rangle]+\frac{1}{2}Z^i(\bar{1}\bar{x},\bar{2}\bar{y})\langle\{R_{z,1},R_2\}_u\rangle+\frac{1}{2}U^i(\bar{x}\bar{1}\bar{2},\bar{y})r(z,u12)=0, \quad (83)$$

where

$$\begin{aligned}U^i(\bar{x}\bar{1}\bar{2},\bar{y})=r_i(\bar{x}\bar{1}\bar{2},\bar{y})+\frac{1}{4}r_i(\bar{x},\bar{1}\bar{2}\bar{y})-\frac{1}{2}\langle\{\tilde{R}_{\bar{x},\bar{y}}{}^i,\tilde{R}_{\bar{1}\bar{2}}{}^i\}^i\rangle\\ -\frac{1}{2}\langle\{R_{\bar{x}},\tilde{R}_{\bar{1}\bar{2},\bar{y}}{}^i\}^i\rangle-\frac{i}{4}\langle[\tilde{R}_{\bar{x},\bar{y}\bar{1}}{}^i,R_{\bar{2}}]^i\rangle\\ -\frac{i}{4}\langle[R_{\bar{x},\bar{1}},R_{\bar{2},\bar{y}}]^i\rangle-\frac{i}{4}\langle[\tilde{R}_{\bar{x},\bar{y}\bar{2}}{}^i,R_{\bar{1}}]^i\rangle\\ -\frac{i}{4}\langle[R_{\bar{x},\bar{2}},R_{\bar{1},\bar{y}}]^i\rangle-\frac{1}{2}\langle\{\tilde{R}_{\bar{x},\bar{y}}{}^i,(R_{\bar{1}}R_{\bar{2}})\}^i\rangle\\ -\frac{1}{2}\langle\{R_{\bar{x}},(R_{\bar{1}}R_{\bar{2}})_y\}^i\rangle \quad (84)\end{aligned}$$

in analogy to (21).

There exist many more linear homogeneous relations between quantities like those considered. For example, from (61) we derive by ordinary differentiation

$$R_{zu,xy}=\hat{R}_{zu,xy}{}^i+\frac{1}{2}r_i(\bar{1}\bar{2},xy)R_{zu,12}+r_i(\bar{1},xy\bar{2})R_{zu2,1}, \quad (85)$$

where $\hat{R}_{zu,xy}{}^i$ is similar to, but not identical with, $\tilde{R}_{zu,xy}{}^i$ because of a different irreducibility condition.

On defining

$$\begin{aligned}\tilde{Y}_{(\bar{1}\bar{2},\bar{x}\bar{y})}{}^i=r_i(\bar{1},\bar{2}\bar{x}\bar{y})-r_i(\bar{2},\bar{1}\bar{x}\bar{y})-i\langle[R_{\bar{1},\bar{y}},R_{\bar{2},\bar{x}}]^i\rangle\\ -i\langle[\hat{R}_{\bar{1},\bar{x}\bar{y}}{}^i,R_{\bar{2}}]^i\rangle-i\langle[R_{\bar{1},\bar{x}},R_{\bar{2},\bar{y}}]^i\rangle\\ -i\langle[R_{\bar{1}},\hat{R}_{\bar{2},\bar{x}\bar{y}}{}^i]^i\rangle \quad (86)\end{aligned}$$

and

$$\begin{aligned}\tilde{Z}^i(\bar{1}\bar{2},\bar{x}\bar{y})=r_i(\bar{1}\bar{2},\bar{x}\bar{y})-\frac{1}{2}\langle\{R_{\bar{1},\bar{x}},R_{\bar{2},\bar{y}}\}^i\rangle\\ -\frac{1}{2}\langle\{\hat{R}_{\bar{1},\bar{x}\bar{y}}{}^i,R_{\bar{2}}\}^i\rangle-\frac{1}{2}\langle\{R_{\bar{1},\bar{y}},R_{\bar{2},\bar{x}}\}^i\rangle\\ -\frac{1}{2}\langle\{R_{\bar{1}},\hat{R}_{\bar{2},\bar{x}\bar{y}}{}^i\}^i\rangle \quad (87)\end{aligned}$$

we obtain from

$$R_{zu,xy}=\frac{1}{2}\{R_z,R_u\}_{xy}$$

[42] Equation (79) is easily derived from (18) and (19). The index of the brackets denotes differentiation of the whole brackets.

the equation

$$\frac{i}{4}\tilde{Y}^i(\overline{12},\bar{x}\bar{y})\langle[R_{z,1},R_{u,2}]\rangle$$

$$-\frac{1}{2}\tilde{Z}^i(\overline{12},\bar{x}\bar{y})\langle\{R_{z,1},R_{u,2}\}\rangle=0. \quad (88)$$

Discussion of Results

In all the definitions (76), (77), (78), (84), (86), (87), the right-hand side would vanish if the irreducibility sign were absent. Thus, these equations are the two-particle analogs of (48) and similar equations easily obtainable in the one-particle case, provided we can show that the left hand sides X^i etc., vanish and that the "irreducible" brackets actually have that meaning.

We did not succeed in strictly excluding the possibility of a nontrivial solution of the linear homogeneous equations (80), (81), (82), (83), (86), which are analogous to (59) but cannot be solved in the same way.[43] However, one can derive still more equations restricting the quantities X^i etc. For instance, it was found that a method analogous to the first one of the foregoing section, resulting in (47), leads to an equation between Y^i and Z^i, containing linear and bilinear terms. In this case, however, the calculation is considerably more cumbersome than that one of the appendix.

The explanation of this fact that, in whatever way one proceeds, the trivial solution $X^i=Y^i=Z^i=\cdots=0$ remains, has been mentioned in the introduction, namely that the renormalized perturbation theoretical solution (and, in a still more formal sense,[44] even the unrenormalized one) is a formal solution of the system (9) or (12), (18), and it was the structure of that solution which we took as a guide in setting up the Bethe-Salpeter equations of this section. Our findings not only show that the "trivial" solution is a consistent one, but strongly suggest that it is the only possible solution of the nonlinear system as far as the two-particle singularities are concerned, or at least the only solution of physical interest. We hope that further analysis will decide this question. In any case, if the system (80) etc., admits only the trivial solution in lowest order of J, this is so in all orders, as is seen by taking functional derivatives.

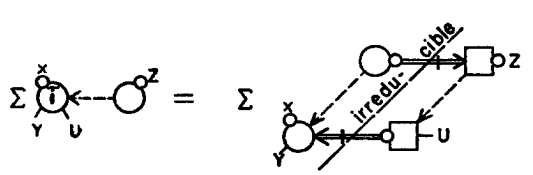

FIG. 8. Two-particle reducibilities of $\langle\{\tilde{R}_{\bar{1},\bar{z}y}{}^i,R_{\bar{x}}\}_c\rangle$, Eq. (A.2).

[43] See, however, note added in proof.

[44] Note that if entirely formal manipulations with singular functions are considered satisfying (25) solves (9) with H_w being any polynomial.

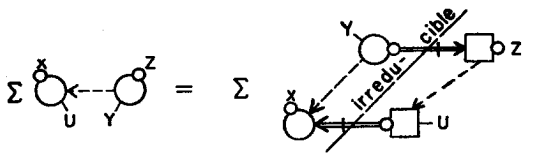

FIG. 9. Two particle reducibilities of $\langle\{R_{x,u},R_{y,z}\}_c\rangle$, Eq. (A.3).

Irreducible Brackets

The meaning of the symbol i at all commutators and anticommutators in (76), (77), (78), (84), (86), and (87) is strictly defined by integral equations of the type (A.2), (A.3), (A.5), (A.6) etc., of the appendix A, and is discussed at the end of that appendix. The result is that it corresponds to picking out of the ordinary brackets the two-particle irreducible parts as described in the following.

Note that all those brackets have the property called $\mathcal{I}$, that they do not allow a cut that separates x, y and 1, 2 from each other and cuts only either two lines (in the sense of the Bethe-Salpeter equations of this section) in one of the two factors, or one line in one factor and a free-particle (contraction) line. This is trivial for brackets like $\langle[R_{\bar{1},\bar{y}},R_{\bar{x},\bar{z}}]\rangle$ and follows from (72) and the definition of the irreducible factors for brackets like

$$\langle\{\tilde{R}_{\bar{1},\bar{z}\bar{y}}{}^i,R_{\bar{z}}\}\rangle, \quad \langle\{\tilde{R}_{\bar{1},\bar{z}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i\}\rangle, \quad \text{and} \quad \langle[(R_{\bar{1}}R_{\bar{2}}),\tilde{R}_{\bar{x},\bar{y}}{}^i]\rangle.$$

Thus, two-particle cuts can only be of the type illustrated by the examples of Figs. 8 and 9. These graphs describe the vacuum expectation value of brackets evaluated as on the right-hand side of (43). Broken lines stand for contraction functions. The other symbols have the usual meaning, and the one-particle structure investigated in the last section, cf., Fig. 3, has been used. "Irreducible" means that, in order to avoid double-counting, on the upper left from the cut no further two-particle cut should be possible. The two-particle cuts in the graphs are composed of two one-particle cuts of known properties, and thus completely defined.

As shown at the end of appendix A, the explicit form of e.g., $\langle[R_{\bar{x},\bar{1}},R_{\bar{2},\bar{y}}]^i\rangle$ is obtained by stretching out the functionals $\langle R_{x,1}\rangle$ and $\langle R_{2,y}\rangle$ into a chain of any length of alternatively irreducible and reducible functionals, and connecting the irreducible links of one chain with all irreducible links of the other chain by functional differential operators

$$\Sigma\equiv\exp\left[\int\int du'du''\frac{\delta}{\delta J'(\mu')}\times\mathbf{K}_{u'}i\Delta^+(u'-u'')\mathbf{K}_{u''}\frac{\delta}{\delta J''(u'')}\right]$$

such that the whole graph becomes two-particle irreducible, the one-particle-reducible end lines being cut off. An example is given in Fig. 10. All such constructions are to be summed up, and the conjugate complex

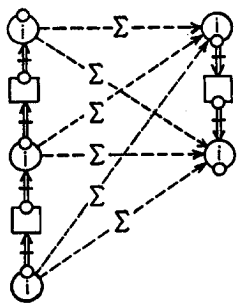

FIG. 10. Contribution to $\langle[R_{\bar{x},\bar{1}},R_{\bar{2},\bar{y}}]^i\rangle$.

quantity subtracted, or added for the anticommutator. The other brackets can be similarly described.

It is important to note that this expansion breaks off for any finite momentum transferred between the two chains, since on each irreducible link must end at least one free-particle line, and all lines have the same frequency sign. Already this shows that this expansion has no relation to perturbation theory but is an expansion in the number of overcrossing groups of contraction lines, which might be called a structure expansion. It directly shows the absence of two-particle singularities (or reducibilities) in the irreducible brackets.

In the appendix it is also pointed out that the sum of all brackets on the right hand side of (77) vanishes if the distance between x and 1 is spacelike, or if at least one of the two coordinates y, 2 is not timelike advanced to at least one of the coordinates x, 1, provided we assume that the solutions of (A.2), (A.3) and similar equations that strictly define the irreducible brackets are unique. The sums of brackets in (76), (78) etc., have similar properties, in concordance with (12).

Decomposition of Other Functionals

On the basis of the considerations which led us finally to (75) we can easily obtain relations for functionals with less than four coordinates. Let us define two functionals $R_{x,\bar{z}\bar{u}}{}^i$ and $R_{x\bar{z},\bar{u}}{}^i$ by the equations

$$R_{x,\bar{z}\bar{u}}=R_{x,\bar{z}\bar{u}}{}^i+\frac{1}{2}r(x,12)R_{\bar{1}\bar{2},\bar{z}\bar{u}}{}^i+r'(x1,2)R_{\bar{2},\bar{1}\bar{z}\bar{u}}{}^i \quad (89)$$

and

$$R_{x\bar{z},\bar{u}}{}'=R_{x\bar{z},\bar{u}}{}^i+\frac{1}{2}r(x,12)R_{\bar{1}\bar{2}\bar{z},\bar{u}}{}^i +r'(x1,2)R_{\bar{2}\bar{z},\bar{1}\bar{u}}{}^i, \quad (z_0<u_0), \quad (90)$$

where the notation has the usual meaning. The vacuum expectation values can be written in the symbolic form

$$G=G_i+G'F_i, \quad (91)$$

where $G'=\{(1/\sqrt{2})r(x,zu),r'(xz,u)\}$ and F_i has the same meaning as in (65) and thereafter. With (73) we obtain from (91) by right multiplication by $1'+'F'$,[45]

$$G'=G_i'+G_i'F'. \quad (92)$$

[45] The possibility of calculations like these, based on (73), were the reason why we started our analysis by discussing the functionals with four, and not with less, coordinates.

This can further be manipulated similarly as mentioned a few lines after (75) to give the two equations

$$R_{x,zu}=\tilde{R}_{x,zu}{}^i+\frac{1}{2}r_i(x,\bar{1}\bar{2})R_{12,zu}+r_i(x\bar{1},\bar{2})R_{2,1zu} \quad (93)$$

and

$$R_{xz,u}{}'=\tilde{R}_{xz,u}{}^i+\frac{1}{2}r_i(x,\bar{1}\bar{2})R_{12z,u}+r_i(x\bar{1},\bar{2})R_{2z,1u}, \quad (z_0<u_0), \quad (94)$$

with a similar property of the $\tilde{R}^i$ functionals as in (72).

From (89), (90), (93), and (94), equations similar to (77) and (78) can be derived. The result is that in both equations the coordinate 2 is to be omitted, and the replacement $1\to x$, $x\to z$, $y\to u$ to be made. There is no essential change in the definition of the irreducible brackets.

Finally, we define a functional $R_{x,y}{}^i$ by

$$R_{x,y}=R_{x,y}{}^i+\frac{1}{2}r_i(x,\bar{1}\bar{2})R_{12,y}{}'+r_i(x\bar{1},\bar{2})R_{2,1y}$$

$$=R_{x,y}{}^i+\frac{1}{2}r(x,12)R_{\bar{1}\bar{2},y}{}^i+r'(x1,2)R_{\bar{2},\bar{1}y}{}^i, \quad (95)$$

(to be used at least once differentiated), where $R_{12,y}{}^i$ is defined by an equation similar to (89). With use of the foregoing results for the other irreducible functionals, $r_i(x,y)$ can be shown, by the usual method, to satisfy an equation that arises from (77) by the replacement $1\to y$, 2 and y omitted, the left-hand side being linear in the "remainders," corresponding to Y, Z, $\tilde{Y}$, $\tilde{Z}$ in (77), (78), (86), and (87), of the functionals with three coordinates.

4. MANY-PARTICLE STRUCTURE

The analysis of the two-particle singularities is in principle extendible, in a straightforward way, to higher singularities. The general type of an n particle singularity is, with $z=p^2-(nm)^2$, $(-z)^{(3n-5)/2}$ if n is even, and $(-z)^{(3n-5)/2}\ln(-z)$ if n is odd, for the case of $m\geqslant 1$ retarded and $n-m$ $\Delta_1/2$ lines on the cut. The terms with as well retarded as advanced lines are not singular, but must be separated out also. The factor in an ansatz similar to (60) of a term with m retarded or $\Delta_1/2$ lines and $n-m$ advanced lines is $[m!(n-m)!]^{-1}R_{\bar{1}\ldots\bar{m},\bar{m}+\bar{1}\ldots\bar{n}zu\ldots}{}^i$. Since, however, the calculations are expected to be, until a simpler calculus is found, considerably more lengthy than in the two-

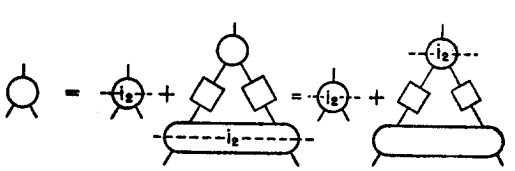

FIG. 11. Analysis of $\langle R_{x,zu}\rangle$, Eqs. (95) and (90).

particle case, but not to present any other difficulty, we take it for granted that the result will be analogous to those of the last two sections.

Rather, we would like to show what such results, together with those of the foregoing sections, do imply. Let us insert (42) and a similar equation for $r(x1,2)$ into (89). This leads to the equation described, together with (93), by Fig. 11, where we draw all lines equal, a summation over all distributions of lines and earliest vertices compatible with the external ones being understood, and only functionals that are one-particle irreducible with respect to the exhibited coordinates (but not yet necessarily with respect to pairs of coordinates) are meant by circles and ovals. The symbol i_2 and the broken line indicate the two-particle irreducibility condition for the fourpoint and threepoint functionals. Separating out the one-particle irreducible part in the first four pointfunctional leads, as one can show, to Fig. 12, which upon neglect of the last term and setting J equal to zero describes a well-known nonlinear integral equation for the threepoint function, the irreducible function, and the twopoint function being considered known. For the irreducible functional, integral equations of the type shown in Fig. 13 will hold.

One easily sees that one can reproduce the perturbation theoretical structure in any detail with, however, a few important differences:

A. One never arrives at a bare vertex. All vertices are still retarded functionals (or, with $J=0$, functions) with certain irreducibility conditions in the sense explained in the last two sections. Formally, in quantum electrodynamics, a vertex that is two-particle irreducible with respect to any external line is necessarily a three-leg point, such that Fig. 13 reduces to a triviality. However, this is not really so because of the need of subtractions in defining the real part from the imaginary part whose decomposition decides the irreducibility test. In the next section we shall give arguments why we do not expect a subtraction to be needed in the present scheme, in contrast to perturbation theory. Instead, in this scheme arbitrarily highly irreducible vertices will exist when it is formulated for quantum electrodynamics. Thus, the freedom gained in the present more general formulation leads at first to the loss of an understanding of the absence of an intrinsic anomalous magnetic moment of the electron. We hope, however, that future study of the consistency of these systems of equations will clear up this point. (See also note added in proof.)

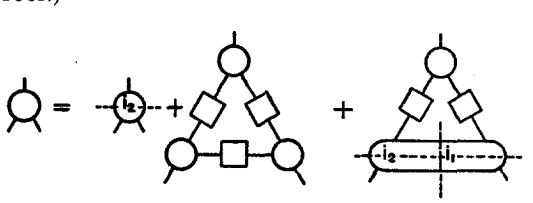

FIG. 12. Further analysis of $\langle R_{x,\,zu}\rangle$.

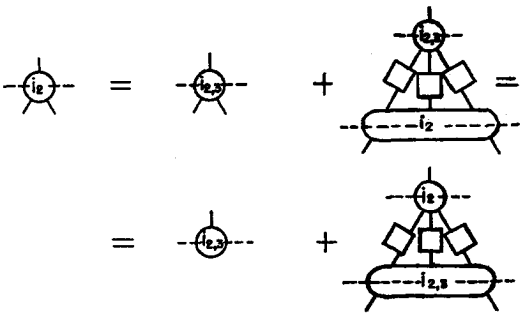

FIG. 13. Analysis of $\langle R_{x,\,zu}{}^{i}\rangle$.

B. One can understand the structure revealed by our analysis as originating from partial summations in double (as in Feynman) graphs containing bare vertices with an arbitrary number of legs.[44] One easily convinces oneself that if one tries to cast the essence of the structure of such graphs into drawings without drawing a potentially infinite number of lines as they were needed in depicting Schwinger's functional differential equation (22), one necessarily arrives at the drawings of generalized Bethe-Salpeter structures shown here, which differ from drawings of Schwinger's equations[46] by the replacement of bare vertices by higher irreducible ones.

Thus, the present scheme leads, upon iteration of the procedure of picking out reducible parts as in the examples of Figs. 12 and 13, to a "structure expansion" with a definite similarity to a perturbation theoretical expansion; the bare vertices, however, are replaced by "causal form factors" related to, but more general than the self energies and vertex parts of the renormalized expansion. Causality is preserved since these "form factors" are again r functionals, merely with an irreducibility condition.[47] This condition has, in a broad sense, the effect of rendering these form factors the less extended in space-time the higher the irreducibility, because of the absence of the low masses in the spectral decomposition of the absorptive parts; that is, of the functions obtained by omitting certain step functions. This effect is seen at the well-known spatial decrease of the vacuum expectation values of ordinary field operator products, which is exponential with a range derived from the lowest masses in the intermediate states,[48] and at the then more rapid oscillation in timelike directions. Thus, as far as low-energy phenomena are concerned, the highly irreducible vertices act similarly as point vertices with, however, a high-energy cutoff, as was already made use of at the beginning of Sec. 3. We shall come back to this important point in the next section.

[46] See, e.g., B and S, p. 430; and R. Utiyama, S. Sunakawa, and T. Imamura, Progr. Theoret. Phys. 8, 77 (1952).

[47] It should be clear that these form factors have as little to do with the form factors of a nonlocal theory as the vertex part, or any generalized vertex obtained by partial summation, of a renormalized local theory has.

[48] R. Haag, Phys. Rev. **112**, 669 (1958). See also G. F. Dell'Antonio, P. Gulmanelli, Nuovo cimento **12**, 38 (1959); and H. Araki (preprint).

Conversely, perturbation theory can be looked at as a degenerate structure expansion. This view would explain its moderate success in certain applications even to strong interactions as, for instance, in pion-nucleon physics,[49] however, more recently described as "pologological." The difficulty one would encounter in quantum electrodynamics has already been mentioned, however, one could also think of pecularities of this very special type of interaction.

Finally, we would like to repeat that in spite of their irreducibility, vertices in the generalized graphs may have any number of external coordinates. Especially, by taking functional derivatives, an arbitrary number of lines external with respect to the whole functional that is analyzed will be set free.[27] Of course, setting $J=0$ gives ordinary graphs, whereupon, for instance, the squares in Fig. 12 reduce to Δ_{Ret}'-functions.

5. STRENGTH OF SINGULARITIES

In the last two sections there appear various integrals that at first sight seem to diverge. Actually, all integrals would do so for $J=0$ in renormalizable perturbation theory, starting at (60). In order to grant these expressions a meaning, an investigation of the behavior of the functions at high momenta is necessary.

One-Particle Propagator[50]

First note that Δ_{Ret}' is restricted only by (49), which serves as its definition, and not by (95) because of (37). In all formulas except (49) Δ_{Ret}' is considered known. Let us rewrite that formula more explicitly as

$$-\Delta_{\mathrm{Av}}'(x-y)+\Delta_{\mathrm{Ret}}'(x-y)+\Delta(x-y)$$
$$=\int\int dx'dy'\Delta_{\mathrm{Ret}}'(x-x')\Pi(\bar{x}'-\bar{y}')\Delta_{\mathrm{Ret}}'(y-y'),$$

where $\Pi(\bar{x}'-\bar{y}')$ is a real odd function. By Fourier transformation we obtain

$$-\tilde{\Delta}_{\mathrm{Av}}'(p)+\tilde{\Delta}_{\mathrm{Ret}}'(p)-2\pi i\epsilon(p_0)\delta(p^2-m^2)$$
$$=2\pi i\tilde{\Delta}_{\mathrm{Ret}}'(p)\tilde{\Pi}(p^2)\tilde{\Delta}_{\mathrm{Av}}'(p)\epsilon(p_0), \quad (96)$$

where $\tilde{\Pi}(p^2)$[51] is real, vanishes for $p^2<4m^2$ up to Dirac delta functions, and is nonnegative for $p^2\geq 4m^2$.

Actually, in the axiomatic scheme, the primary quantity is not $\tilde{\Pi}(p^2)$, but

$$\tilde{\Pi}(p^2)\,|\tilde{\Delta}_{\mathrm{Ret}}'(p)|^2\equiv\rho(p^2), \quad (97)$$

though it might be the other way round in a scheme to solve the whole system (48). Thus, the actual definition of $\tilde{\Pi}(p^2)$ will depend on $\tilde{\Delta}_{\mathrm{Ret}}'(p)$. According to Hall and Wightman,[52] $\tilde{\Delta}_{\mathrm{Ret}}'(p)=\tilde{\Delta}_{\mathrm{Av}}'(-p)$ is a function of p^2 and the boundary value of a single function $f(z)$, which is analytic in the cut $z=p^2$ plane apart from a pole at $z=m^2$, on the upper or lower side of the cut, respectively, if $p_0\gtrless 0$. Equation (96) can be rewritten

$$f(x+i0)-f(x-i0)=2\pi i\delta(x-m^2)+2\pi i\theta(x-4m^2)\rho(x).$$

The function $f(z)$ can be defined by

$$f(z)=\frac{1}{m^2-z}+\int_{4m^2}^{\infty}dt\frac{\rho(t)}{t-z} \quad (99)$$

in the usual way, if this integral exists. Then $f(z)$ has positive imaginary part in the upper z half plane, vanishes in infinity in every direction not parallel to the positive real axis, and vanishes at most at one real point x_0 between m^2 and $4m^2$, and at a possibly infinite number of real discrete points $x_\nu>4m^2$, $\nu=1\cdots$. At these zeros the real part of $f(x)$ will have positive slope and the function $\tilde{\Pi}(x)$ will be defined only up to a delta function with positive coefficient.[53]

If the integral in (99) does not exist, subtractions[54] will be necessary in order to arrive at a definition of $f(z)$. These are, for our purpose, most conveniently carried out by defining

$$f(z)=g(z)\prod_{l=1}^{L}\frac{z-x_l}{m^2-x_l}\equiv g(z)Q(z), \quad (100)$$

where the x_l are real and between 0 and m^2. By using (100) in (98) we obtain as a possible definition of $f(z)$,

$$f(z)=Q(z)\left[\frac{1}{m^2-z}+\int_{4m^2}^{\infty}dt\frac{\rho(t)}{Q(t)(t-z)}\right], \quad (101)$$

where the bracket $g(z)$ has the same properties as (99). Because of the above choice of the zeros of $Q(z)$, the amputation defined in Sec. 2 and often used later remains a well-defined operation, since at all those zeros the retarded (or advanced) boundary condition, whose observation was always implied, gives a unique definition. (See, however, note added in proof.)

The exceptional case is (49) or (96) itself, if not $\rho(p^2)$ but $\tilde{\Pi}(p^2)$ is considered the primary quantity. We shall show in the appendix that if we do not permit nonCDD zeros, we have the representation

$$f(z)=(m^2-z)^{-1}\left[B+\int_{4m^2}^{\infty}dt\frac{\tilde{\Pi}(t)}{(t-z)(t-m^2)}+\sum\frac{C_\lambda}{(x_\lambda-z)(x_\lambda-m^2)}\right]^{-1}, \quad (102)$$

[49] See, e.g., R. E. Marshak, *Meson Physics* (McGraw-Hill Book Company, Inc., New York, 1952).

[50] The following analysis is mainly a generalization of that of footnote 8.

[51] $2\pi\tilde{\Pi}(p^2)$ is identical with the function $F(-p^2)$, the absorptive part of Dyson's proper self energy part, of footnote 8.

[52] D. Hall and A. S. Wightman, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **31**, No. 5 (1957).

[53] For a thorough discussion see L. Castillejo, R. H. Dalitz, and F. J. Dyson, Phys. Rev. **101**, 453 (1956). We shall refer to zeros with these properties for brevity as CDD zeros.

[54] See, e.g., B and S, p. 587.

where B is real nonnegative, the x_λ are real, the C_λ positive, and

$$B+\int_{4m^2}^{\infty} dt\frac{\tilde{\Pi}(t)}{(t-m^2)^2}+\sum\frac{C_\lambda}{(x_\lambda-m^2)^2}=1. \quad (103)$$

Comparison with (99) gives

$$B^{-1}=1+\int_{4m^2}^{\infty}\rho(t)dt.$$

If $B=0$, we obtain

$$f(z)\to\left[\int_{4m^2}^{\infty}\frac{\tilde{\Pi}(t)dt}{t-m^2}+\sum\frac{C_\lambda}{x_\lambda-m^2}\right]^{-1} \quad (104)$$

if $z\to\infty$, such that in this case, if (99) should apply, the sum, or integral, or both, in (104) must diverge, since otherwise in (99) a constant corresponding to (104) would have to be added.

Thus, unless

$$I\equiv\int_{4m^2}^{\infty} dt\frac{\tilde{\Pi}(t)}{(t-m^2)^2}\leq 1 \quad (105)$$

there cannot exist a representation of the type (99). If $I<1$, one may choose a finite B, or CDD zeros, or both, such as to satisfy (103) and to make (104) vanish if we decide for $B=0$. $f(z)$ is defined by (102).

We shall show in the appendix that if $I>1$ but $\tilde{\Pi}(t)=0(t^{-1})$ in infinity, one might possibly find, in any case if $\tilde{\Pi}(t)$ vanishes stronger than any negative power of t, a subtracted form of $f(z)$ that belongs to that $\tilde{\Pi}(t)$, by choosing sufficiently many nonCDD zeros. If, however, I does not exist there is no way to define a function $f(z)$, with only polynomial growth in infinity, that gives $\tilde{\Pi}(t)$. This is the irreparable "ghost" situation.

The "normal" situation is that considered before, namely $I\leq 1$. We saw that if (99) should hold with $I=1$, the integral and sum together in (104) will diverge, which means that in (49) we cannot obtain $\Delta_{\text{Ret}}''(\bar{x}-\bar{y})$ by multiplying (49) by $\theta(x-y)$, but that one subtraction is required. Actually, the data for two subtractions are available, as insertion of (103) into (102) shows. This is the situation in renormalizable perturbation theory, where $\tilde{\Pi}(t)$ increases in infinity like $t(\ln t)^\mu$, $\mu\geq 0$, and (102) is not applicable. We find that permitting subtracted forms of $f(z)$ does not help here.

If $I<1$ there are various choices for unsubtracted $f(z)$, as (103) and (102) show. The former conclusion on the stepfunction multiplication only holds if we decide for $B=0$, and the divergence of (104) is not due to CDD zeros, which, however, can hardly be expected to be separable from the $\tilde{\Pi}(t)$-determination.

Other Functions

The finding that for a consistent theory of the type considered in the axiomatic scheme, the strength of the singularity of an Δ_{Ret}'-amputated function is less than in renormalizable perturbation theory is of great interest. Whereas we can prove it only for the absorptive irreducible part of the propagation function itself and for the vertex function with two momenta on the mass shell,[50] we conjecture it to be true for all functions. This would imply that for the vertex function where in perturbation theory, independent of Δ_{Ret}- or Δ_{Ret}'-amputation, one subtraction is necessary, in our treatment no subtraction would be required,[55] and that all Δ_{Ret}'-amputated functions could be obtained[56] from the absorptive parts by multiplication of (48) by the step function.

Let us relate these considerations to renormalization theory. Consider, for instance, the usual pseudoscalar meson theory with, among others, the coupling term

$$g_u\bar{\psi}_u\gamma_5\tau^i\psi_u\phi_u{}^i$$

in unrenormalized, or

$$Z_1g_r\bar{\psi}_r\gamma_5\tau^i\psi_r\phi_r{}^i$$

in renormalized quantities, because of

$$\psi_u=Z_2^{\frac{1}{2}}\psi_r,\quad \bar{\psi}_u=Z_2^{\frac{1}{2}}\bar{\psi}_r,\quad \phi_u{}^i=Z_3^{\frac{1}{2}}\phi_r{}^i,\quad g_u=Z_1Z_2^{-1}Z_3^{-\frac{1}{2}}g_r.$$

Arguments[57] can be given for the validity of the Born approximation at high energies. For the vertex part the Born approximation is obtained by taking in

$$\int du\langle T\psi_r(x)\bar{\psi}_r(y)\phi_r{}^i(z)Z_1g_r\bar{\psi}_r(u)\gamma_5\tau^i\psi_r(u)\phi_r{}^i(u)\rangle$$

the disconnected part, which gives

$$Z_1g_r\int du S_F'(x-u)\gamma_5\tau^i S_F'(u-y)\Delta_F'(u-z).$$

Thus, the amputated vertex behaves like $Z_1g_r\gamma_5\tau^i$ in infinity, which also holds if two of the particle momenta are on the mass shell, the third one going to infinity.[58] Comparison with the results on the meson propagation function[50] shows that $Z_1=0$.[59] We thus find that the Δ_{Ret}'-amputated vertex function goes to zero in infinity

[55] A similar conjecture has been brought forward by G. F. Chew, UCRL-8194, in connection with the electromagnetic structure problem of the nucleon.

[56] This was suggested to the author by F. J. Dyson.

[57] G. Källen, in "Quantum electrodynamics," Encyclopedia of Physics, Vol. 5, part I, p. 302 (Springer Verlag, Berlin, Germany, 1958); CERN 57-43. See also K. Symanzik, Nuovo cimento 11, 269 (1959).

[58] Note that use of a dispersion relation for the vertex in a form that is proven (e.g., in the meson-nucleon vertex keep a nucleon momentum off the mass shell) gives a definition for Z_1 similar to the well-known definitions of Z_2, Z_3, and the self masses in terms of integrals over spectral functions, e.g., H. Lehmann, Nuovo cimento 11, 342 (1954).

[59] In quantum electrodynamics, because of Ward's identity, this leads to $Z_2=0$. This argument has been used by G. Källen, (footnote 57), to identify one vanishing renormalization constant in quantum electrodynamics if one adheres to Dyson's perturbation-theoretical renormalization scheme, but does not use the expansion in powers of the charge.

also when more than one momentum is off the mass shell, in accordance with the conjecture described above.

On the basis of that conjecture, we can argue for the existence of the integrals of the last two sections. Since they are at most logarithmically divergent in perturbation theory, they will become convergent since the gain in convergence discussed above for the vertex, which is at least by powers of logarithms can be expected sufficient.

It seems that the arguments collected here lend support to the view that the strength of singularities in renormalized perturbation theory is an upper bound, which is, in fact, not reached by a rigorous solution of the axiomatic scheme, at least as far as the Δ_{Ret}'-amputated functions are concerned. The singularities (or vertex divergencies) in perturbation theory seem to be characteristic to that method, which is strict in locality but loose in unitarity.

6. OUTLOOK

The results of the foregoing sections can be utilized to amend present methods to derive analytic properties of

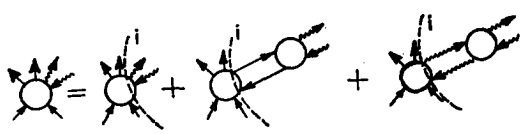

FIG. 14. Analysis of the scattering amplitude $A+A \rightarrow A+A+a+\bar{a}$.

observable quantities because structure analysis permits use of locality and the completeness condition more efficiently than techniques presently available do.

This is most easily seen by comparison of field theoretical proofs of analytic properties of scattering amplitudes with proofs for potential scattering. Lehmann's proof[60] of $\cos\theta$-analyticity for fixed total energy gives as analyticity region an ellipse, which is analogous to the ellipse obtained by Khuri[61] for potentials that are local and decrease exponentially, but are not restricted otherwise. Blankenbecler *et al.*[62] have shown that the initial ellipse can be successively enlarged, if the potential is a superposition of Yukawa potentials, by iteration of the integrated Schrödinger equation, whereby the Born series is generated.

We may compare the Schrödinger equation to the inhomogeneous Bethe-Salpeter equation of Fig. 7 and, especially, Eq. (69). Actually, the ladder approximation of the Bethe-Salpeter equation was originally proposed by Nambu[63] as field theoretical analog of the Schrödinger equation and is known to lead to it in the nonrelativistic adiabatic approximation. In Lehmann's

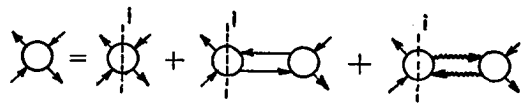

FIG. 15. Analysis of $A+\bar{A} \rightarrow A+\bar{A}$, Eq. (106).

proof[60] of $\cos\theta$-analyticity, the "Yukawa-type" nature of the "potential," namely that it is originated by the causal interaction of particles with known mass spectrum, is used only once, comparable to terminate the iteration mentioned in the foregoing with the first or, for the absorptive part, second Born approximation.

As far as the dispersion relation for fixed momentum transfer $|\Delta|$ is concerned, for limited $|\Delta|$ the irreducible term in Fig. 7 has zero absorptive part in the unphysical region $|\omega| < (m^2+\Delta^2)^{\frac{1}{2}}$, as follows from (77) with $Y^i=0$, and therefore obeys a homogeneous dispersion relation. The reducible part, however, must be analyzed on the basis of its structure. Since it resembles, in its iterated form, a perturbation theoretical graph with, however, vertices of finite but, in comparison with the reducible functions, reduced extent (if, for instance, a further analysis like that of Fig. 12 is carried out), it can be expected that techniques developed for proofs of analytic properties of Feynman graphs can be adapted to the present situation.

In the case of meson-nucleon forward scattering, Zimmermann[64] has shown that already separating out the one-nucleon reducible part permits proving the dispersion relation and identifying the coupling constant in a simple way.

These considerations, together with the remarks about a possible interpretation of perturbation theory in Sec. 4, might lead in the direction of Landau's[65] recent method. The method proposed here has in common with this at least that all stable particles, without a distinction between "simple" and "composite" ones, are treated equally. Here, this is clearly based on Zimmermann's[66] technique of ascribing local field operators to all stable particles.

This leads us to the question why it is obviously sometimes advantageous to treat an unstable particle like a stable one, since a neglect of the decay interaction cannot be spoken about when bare interactions do not appear at all. A justification is desirable because even apparently stable particles might be unstable with a long lifetime.

Of course, we are not in a position to give anything else than a very crude qualitative argument. Assume a

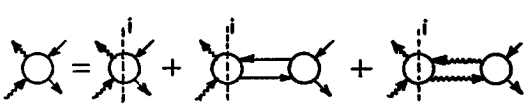

FIG. 16. Analysis of $a+\bar{a} \rightarrow A+\bar{A}$, Eq. (107).

[60] H. Lehmann, Nuovo cimento **10**, 579 (1958).
[61] N. N. Khuri, Phys. Rev. **107**, 1148 (1957). See also S. Gasiorowicz and H. P. Noyes, Nuovo cimento **10**, 78 (1958).
[62] R. Blankenbecler, M. L. Goldberger, N. N. Khuri, and S. B. Treiman (to be published).
[63] Y. Nambu, Progr. Theoret. Phys. **5**, 614 (1950).
[64] W. Zimmermann, Nuovo cimento **13**, 503 (1959).
[65] L. D. Landau, Nuclear Phys. **13**, 181 (1959).
[66] W. Zimmermann, Nuovo cimento **10**, 597 (1958).

model[67] with stable particles A, antiparticles $\bar{A}$, and lighter stable particles a, and antiparticles $\bar{a}$, and as well A- as a-conservation. The scattering amplitude $A+A\to A+A+a+\bar{a}$ can be structure-analyzed as shown[68] in Fig. 14, where i denotes one- and two-particle irreducibility. Furthermore, the integral equations described by Figs. 15 and 16 are written symbolically as

$$X=X_i+X_iX+Y_i{}^TY \tag{106}$$

and

$$Y=Y_i+Y_iX+Z_iY, \tag{107}$$

respectively, where integrations over the relative coordinates are implied. If Z_i can be neglected, we obtain[69]

$$Y=Y_i[1-X_i-Y_i{}^TY_i]^{-1}$$
$$=Y_i[1-X_i]^{-1}[1-Y_i{}^TY_i(1-X_i)^{-1}]^{-1},$$

which gives the final-state interaction in the middle graph of Fig. 14. If at some momentum in the energy region between $2m_A$ and $2m_a$ X_i, being there a hermitian operator, having (for instance in the zero angular momentum channel) the eigenvalue one, with $Y_i{}^TY_i$ being there a small but, of course, nonhermitian operator, a resonance, giving rise to a clean decoupling of the production and the decay process, will appear. To a pair of two a-particles in strong correlation to each other in a large timelike distance only this resonance, phenomenologically described as an unstable particle, will give a measurable contribution.

It is clear that the consideration given here for two end lines also applies to a pair of interior A, $\bar{A}$-lines (more precisely, an interior fourpoint vertex) though the advantage of using the unstable particle as a substitute for that pair will be limited to certain energy regions.

The explanation given here is not new and does not give a hint why resonances that are actually observed are so sharp. However, from a fundamental point of view a hierarchy of interactions, strong and weak ones, is not much easier to understand.

The structure analysis as presented in this paper is an off-shell formalism. We expect that it will be possible to reduce it, by dispersion-theoretical methods, at least partly to an on-shell formalism. It seems to us that on-shell methods, being beset with the problem of unphysical and high-energy regions, can only be understood and adequately handled with a prior comprehension of the underlying off-shell theory, unless a direct approach to the causality problem of the S matrix has been found. Moreover, the technical difficulties of unphysical regions might in some cases become so unwieldy that a complete reduction to the mass shells is no longer advantageous.

[67] We do not choose a more realistic model in order to avoid the impression of an allusion to a quantitative applicability of the following reflections.

[68] The circles denote functions and not functionals. The same simplification as in Figs. 11, 12, and 13 with respect to lines and earliest coordinates are made.

[69] The less simple considerations of Sec. 3 in a similar case are not needed here.

ACKNOWLEDGMENTS

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APPENDIX A

Elimination of the Two-Particle Reducibilities (Section 3)

We insert (68) and (60) on the left and also on the right-hand side of (44), always exhibiting the reducibility between x, y and z, u nearest to x if there is any. The result is

$$\langle\tilde{R}_{x,yzu}{}^i\rangle+\frac{1}{2}r_i(x,y\bar{1}\bar{2})\langle R_{12,zu}\rangle+r_i(x\bar{1},y\bar{2})\langle R_{2,1zu}\rangle$$
$$-\frac{1}{2}r(z,u12)\langle R_{\bar{1}\bar{2},xy}{}^i\rangle-r(z1,u2)\langle R_{\bar{2},\bar{1}xy}{}^i\rangle$$
$$=i\langle[\tilde{R}_{x,yu}{}^i,R_z]\rangle+i\langle[R_{x,u},R_{z,y}]\rangle$$
$$+\frac{i}{2}[\langle[\tilde{R}_{x,y}{}^i,R_{\bar{1}\bar{2}}{}^i]\rangle+\langle[R_x,R_{\bar{1}\bar{2},y}{}^i]\rangle]r(z,u12)$$
$$+i[\langle[\tilde{R}_{x,y}{}^i,R_{\bar{2},\bar{1}}{}^i]\rangle+\langle[R_x,R_{\bar{2},\bar{1}y}{}^i]\rangle]r(z1,u2)$$
$$+\frac{i}{2}r_i(x,y\bar{1}\bar{2})\langle[R_{12},R_z]_u\rangle$$
$$+ir_i(x\bar{1},y\bar{2})\langle[R_{2,1},R_z]_u\rangle, \tag{A.1}$$

where all one-particle reducible terms are neglected.

The first two brackets on the right-hand side (rhs) of (A.1) have the property $\mathfrak{s}$ defined in Sec. 3. For such brackets we define the operations $[\ ]^i$ and $\{\ \}^i$ by the integral equations[70]

$$\langle[\tilde{R}_{x,yu}{}^i,R_z]\rangle=\frac{1}{2}\langle[\tilde{R}_{x,y\bar{1}}{}^i,R_{\bar{2}}]^i\rangle\langle\{R_{1,u},R_{z,2}\}\rangle$$
$$+\frac{1}{2}\langle\{\tilde{R}_{x,y\bar{1}}{}^i,R_{\bar{2}}\}^i\rangle\langle[R_{1,u},R_{z,2}]\rangle, \tag{A.2a}$$

$$\langle\{\tilde{R}_{x,yu}{}^i,R_z\}_c\rangle=\frac{1}{2}\langle[\tilde{R}_{x,y\bar{1}}{}^i,R_{\bar{2}}]^i\rangle\langle[R_{1,u},R_{z,2}]\rangle$$
$$+\frac{1}{2}\langle\{\tilde{R}_{x,y\bar{1}}{}^i,R_2\}^i\rangle\langle\{R_{1,u},R_{z,2}\}\rangle, \tag{A.2b}$$

[70] The index c of the anticommutators denotes the connected part, obtained by subtracting the disconnected part, which is, e.g., $2\langle\tilde{R}_{x,yu}{}^i\rangle\langle R_z\rangle$ for (A.2b).

$$\langle[R_{x,u},R_{z,y}]\rangle=\frac{1}{2}\langle[R_{x,\bar{1}},R_{\bar{2},y}]^i\rangle\langle\{R_{1,u},R_{z,2}\}\rangle + \frac{1}{2}\langle\{R_{x,\bar{1}},R_{\bar{2},y}\}^i\rangle\langle[R_{1,u},R_{z,2}]\rangle, \quad \text{(A.3a)}$$

$$\langle\{R_{x,u},R_{z,y}\}_c\rangle=\frac{1}{2}\langle[R_{x,\bar{1}},R_{\bar{2},y}]^i\rangle\langle[R_{1,u},R_{z,2}]\rangle + \frac{1}{2}\langle\{R_{x,\bar{1}},R_{\bar{2},y}\}^i\rangle\langle\{R_{1,u},R_{z,2}\}\rangle, \quad \text{(A.3b)}$$

which correspond to Figs. 8 and 9, since for two operators A, B that commute with the operators C, D the equations

$$[AC,BD]=\frac{1}{2}[A,B]\{C,D\}+\frac{1}{2}\{A,B\}[C,D] \quad \text{(A.4a)}$$

and

$$\{AC,BD\}=\frac{1}{2}[A,B][C,D]+\frac{1}{2}\{A,B\}\{C,D\} \quad \text{(A.4b)}$$

hold. The structure of (A.2) and (A.3) is very similar to that of (68) and (70). We defer the discussion of (A.2) and (A.3) to the end of this appendix.

The brackets in the third and fourth term on the rhs of (A.1) do not yet have the property $\mathcal{I}$, since they contain $R_{\bar{1}\bar{2}}{}^i$ instead of $\tilde{R}_{\bar{1}\bar{2}}{}^i$ etc. By using (72) we write

$$\begin{aligned}\langle[\tilde{R}_{x,y}{}^i,R_{\bar{1}\bar{2}}{}^i]\rangle &=\frac{1}{2}\langle[\tilde{R}_{x,y}{}^i,(R_{\bar{3}}R_{\bar{4}})]\rangle r_i(\overline{12},34)+\langle[\tilde{R}_{x,y}{}^i,\tilde{R}_{\bar{1}\bar{2}}{}^i]\rangle\\ &=\frac{1}{2}\langle[\tilde{R}_{x,y}{}^i,(R_{\bar{3}}R_{\bar{4}})]\rangle r_i(\overline{12},34)\\ &\quad+\frac{1}{2}\langle[\tilde{R}_{x,y\bar{3}}{}^i,R_{\bar{4}}]^i\rangle\langle\{R_3,\tilde{R}_{\bar{1}\bar{2},4}{}^i\}\rangle\\ &\quad+\frac{1}{2}\langle\{\tilde{R}_{x,y\bar{3}}{}^i,R_{\bar{4}}\}^i\rangle\langle[R_3,\tilde{R}_{\bar{1}\bar{2},4}{}^i]\rangle\\ &\quad+\langle[\tilde{R}_{x,y}{}^i,\tilde{R}_{\bar{1}\bar{2}}{}^i]^i\rangle \quad \text{(A.5)}\end{aligned}$$

and

$$\begin{aligned}\langle[R_x,R_{\bar{1}\bar{2},y}{}^i]\rangle &=\frac{1}{2}\langle[R_x,(R_{\bar{3}}R_{\bar{4}})_y]\rangle r_i(\overline{12},34)+\langle[R_x,\tilde{R}_{\bar{1}\bar{2},y}{}^i]\rangle\\ &=\frac{1}{2}\langle[R_x,(R_{\bar{3}}R_{\bar{4}})_y]\rangle r_i(\overline{12},34)\\ &\quad+\frac{1}{2}\langle[R_{x,\bar{3}},R_{\bar{4},y}]^i\rangle\langle\{R_3,\tilde{R}_{\bar{1}\bar{2},4}{}^i\}\rangle\\ &\quad+\frac{1}{2}\langle\{R_{x,\bar{3}},R_{\bar{4},y}\}^i\rangle\langle[R_3,\tilde{R}_{\bar{1}\bar{2},4}{}^i]\rangle\\ &\quad+\langle[R_x,\tilde{R}_{\bar{1}\bar{2},y}{}^i]^i\rangle, \quad \text{(A.6)}\end{aligned}$$

where the last terms in (A.5) and (A.6) are defined by these equations, since the other irreducible brackets have been defined by (A.2) and (A.3). The meaning of the terms separated out first is explained by

$$\langle[\tilde{R}_{x,y}{}^i,(R_{\bar{3}}R_{\bar{4}})]\rangle=\langle\tilde{R}_{x,y}{}^i\rangle\left(\exp\left[\frac{\delta}{\delta J}\mathbf{K}i\Delta^+\mathbf{K}\frac{\delta}{\delta J}\right]-\exp\left[\frac{\delta}{\delta J}\mathbf{K}(-i\Delta^-)\mathbf{K}\frac{\delta}{\delta J}\right]\right)\langle R_{\bar{3}}\rangle\langle R_{\bar{4}}\rangle$$

with differentiations as in (43), as follows from the sense in which (72) was understood. The differentiations of $\langle\tilde{R}_{x,y}{}^i\rangle$ are contraction differentiations and as such again defined with the help of (72). We shall see later that $\langle[R_x,\tilde{R}_{\bar{2},\bar{1}y}{}^i]^i\rangle$ and $\langle[\tilde{R}_{x,yu}{}^i,R_z]^i\rangle$ are closely related. The brackets in the fourth term on the rhs of (A.1) are obtained from (A.5) and (A.6) by the replacement $R_{\bar{1}\bar{2}}{}^i\to R_{\bar{2},\bar{1}}{}^i$.

Equations (A.5), (A.6), and the two equations just described give upon use of (60), (72), and the equation for $\tilde{R}_{\bar{2},\bar{1}}{}^i$ corresponding to (72), for the sum of the third and fourth term on the rhs of (A.1),

$$\begin{aligned}&\frac{i}{2}[\langle[\tilde{R}_{x,y\bar{3}}{}^i,R_{\bar{4}}]^i\rangle+\langle[R_{x,\bar{3}},R_{\bar{4},y}]^i\rangle]\\ &\times\left[\langle\{R_3,R_{z,u4}\}\rangle-\frac{1}{2}\langle\{R_3,(R_{\bar{5}}R_{\bar{6}})_4\}\rangle\cdot r(z,u56)\right]\\ &+\frac{i}{2}[\langle\{\tilde{R}_{x,y\bar{3}}{}^i,R_{\bar{4}}\}^i\rangle+\langle\{R_{x,\bar{3}},R_{\bar{4},y}\}^i\rangle]\\ &\times\left[\langle[R_3,R_{z,u4}]\rangle-\frac{1}{2}\langle[R_3,(R_{\bar{5}}R_{\bar{6}})_4]\rangle r(z,u56)\right]\\ &+\frac{i}{2}[\langle[\tilde{R}_{x,y}{}^i,(R_{\bar{3}}R_{\bar{4}})]\rangle+\langle[R_x,(R_{\bar{3}}R_{\bar{4}})_y]\rangle]r(z,u34)\\ &+\frac{i}{2}[\langle[\tilde{R}_{x,y}{}^i,\tilde{R}_{\bar{1}\bar{2}}{}^i]^i\rangle+\langle[R_x,\tilde{R}_{\bar{1}\bar{2},y}{}^i]^i\rangle]r(z,u12)\\ &+i[\langle[\tilde{R}_{x,y}{}^i,\tilde{R}_{\bar{2},\bar{1}}{}^i]^i\rangle+\langle[R_x,\tilde{R}_{\bar{2},\bar{1}y}{}^i]^i\rangle]r(z1,u2). \quad \text{(A.7)}\end{aligned}$$

For the terms containing the products R_5R_6 or R_3R_4 we define in the usual way,

$$\begin{aligned}\langle[\tilde{R}_{x,y}{}^i,(R_{\bar{5}}R_{\bar{6}})]\rangle &=\frac{1}{2}\langle[\tilde{R}_{x,y\bar{3}}{}^i,R_{\bar{4}}]^i\rangle\langle\{R_3,(R_{\bar{5}}R_{\bar{6}})_4\}\rangle\\ &\quad+\frac{1}{2}\langle\{\tilde{R}_{x,y\bar{3}}{}^i,R_{\bar{4}}\}^i\rangle\langle[R_3,(R_{\bar{5}}R_{\bar{6}})_4]\rangle\\ &\quad+\langle[\tilde{R}_{x,y}{}^i,(R_{\bar{5}}R_{\bar{6}})]^i\rangle \quad \text{(A.8)}\end{aligned}$$

and

$$\langle[R_x,(R_{\bar{5}}R_{\bar{6}})_y]\rangle$$
$$=\frac{1}{2}\langle[R_{x,\bar{3}},R_{\bar{4},y}]^i\rangle\langle\{R_3,(R_{\bar{5}}R_{\bar{6}})_4\}\rangle$$
$$+\frac{1}{2}\langle\{R_{x,\bar{3}},R_{\bar{4},y}\}^i\rangle\langle[R_3,(R_{\bar{5}}R_{\bar{6}})_4]\rangle$$
$$+\langle[R_x,(R_{\bar{5}}R_{\bar{6}})_y]^i\rangle \quad \text{(A.9)}$$

since the lhs brackets have, because of the amputation of the one-particle reducibilities (after the commutator has been worked out, of course), the property $\mathcal{G}$. The other irreducible brackets have been defined in (A.2), (A.3). The interpretation of these decompositions follows the pattern discussed at the end of this appendix.

The remaining parts of the first two terms of (A.7) can be combined with (A.2a) and (A.3a), whereupon the last brackets change into $\langle\{R_3,R_{z,4}\}_u\rangle$ and $\langle[R_3,R_{z,4}]_u\rangle$, respectively.

For the coefficient of the penultimate term on the right-hand side of (A.1) we have from (19) and (18)

$$i[R_{12},R_z]_u=R_{12,zu}-R_{1z,2u}-R_{2z,1u}$$
$$+\frac{1}{2}\{R_{1,2},R_z\}_u+\frac{1}{2}\{R_{2,1},R_z\}_u, \quad \text{(A.10)}$$

whose first term cancels, upon insertion into (A.1), the second term on the lhs of that equation. For the last term in (A.1) we use (18) and obtain

$$i[R_{2,1},R_z]_u=R_{2,1zu}-R_{z,21u}-i[R_2,R_{z,1}]_u \quad \text{(A.11)}$$

whose first term cancels the third term on the lhs of (A.1).

We now define X^i by (76), which was set up in analogy to (A.10) where, however, a moment's thought should be given to the terms containing R_1R_2. They arise from the need of adding to, e.g., $\langle[\tilde{R}_{\bar{1}\bar{2}}{}^i,\tilde{R}_{\bar{x},\bar{y}}{}^i]^i\rangle$ those terms where, before the irreducible commutator was worked out, the first factor was disconnected between 1 and 2. Without that term, the full analogy between (76) and (79) would have been spoiled since $\tilde{R}_{12}{}^i$ contains only between 1 and 2 connected terms, in contrast to R_{12}. This also explains why such additional terms do not appear in Y, $\tilde{Y}$, Z, $\tilde{Z}$, but do in U. All irreducible brackets in (76) have either already been defined earlier, or are defined by the anticommutator equations analogous to (A.5), (A.6), etc. When (76) is used in the penultimate term of (A.7), the first term on the rhs of (76) cancels the fourth term on the lhs of (A.1), and the second and third term cancel the second term on the rhs of (A.11).

If (76) would have been written with unamputated 1, 2, X^i would have little chance to vanish because on the rhs 1 and 2 occur in varying positions, and the conversion of retarded into advanced end reducibilities would have given additional terms.

If we furthermore use (77) for the last term in (A.7), the first term on the rhs of (77) cancels the last term on the lhs of (A.1), and the second term cancels the second and third term on the rhs of (A.10).

Let us collect what remains of (A.1) upon insertion of (A.7) to (A.11), (76), (77), (A.2a) and (A.3a),

$$\langle\tilde{R}_{x,yzu}{}^i\rangle=\frac{i}{2}[\langle[\tilde{R}_{x,y\bar{1}}{}^i,R_{\bar{2}}]^i\rangle+\langle[R_{x,\bar{1}},R_{\bar{2},y}]^i\rangle]$$
$$\cdot[\langle\{R_1,R_{z,2}\}_u\rangle-2r(z1,u2)]$$
$$+\frac{i}{2}[\langle\{\tilde{R}_{x,y\bar{1}}{}^i,R_{\bar{2}}\}^i\rangle+\langle\{R_{x,\bar{1}},R_{\bar{2},y}\}^i\rangle]$$
$$\times\langle[R_1,R_{z,2}]_u\rangle+\frac{1}{2}r_i(x,y\bar{1}\bar{2})\langle\{R_{1,2},R_z\}_u\rangle$$
$$+ir_i(x\bar{1},y\bar{2})\langle[R_{z,1},R_2]_u\rangle$$
$$-\frac{1}{2}[\langle\{R_x,\tilde{R}_{\bar{1},\bar{2}y}{}^i\}^i\rangle+\langle\{\tilde{R}_{x,y}{}^i,\tilde{R}_{\bar{1},\bar{2}}{}^i\}^i\rangle]r(z,u12)$$
$$+\frac{1}{2}X^i(x\bar{1}\bar{2},y)r(z,u12)$$
$$+Y^i(\bar{2}x,\bar{1}y)r(z1,u2). \quad \text{(A.12)}$$

In the third term on the rhs, we have from (77)

$$r_i(x,y\bar{1}\bar{2})=r_i(\bar{2},xy\bar{1})+i\langle[\tilde{R}_{x,y}{}^i,\tilde{R}_{\bar{2},\bar{1}}{}^i]^i\rangle$$
$$+i\langle[R_x,\tilde{R}_{\bar{2},\bar{1}y}{}^i]^i\rangle+i\langle[R_{x,\bar{1}},R_{\bar{2},y}]^i\rangle$$
$$+i\langle[\tilde{R}_{x,y\bar{1}}{}^i,R_{\bar{2}}]^i\rangle-Y^i(\bar{2}x,\bar{1}y).$$

The first three terms on the rhs do not contribute in (A.12) because of the inverse time order of 1 and 2 in the two factors.[71] The fourth and fifth term cancel the first term on the rhs of (A.12). In the fourth term on the rhs of that equation we use (78), all irreducible brackets of which have been defined earlier. The second and third term on the rhs of (78) cancel the second term on the rhs of (A.12), whereas the fourth and fifth term combine with the fifth term on the rhs of (A.12) to give a coefficient

$$i\langle[R_{z,1},R_2]_u\rangle-r(z,u12)=i\langle[R_z,R_{2,1}]_u\rangle,$$

which results in a vanishing term due to inverse time order.[71] Taking account of (72) and combining with (19) the coefficients of Y^i we are left with (80).

The Eqs. (81), (82), (83), (88) are obtained in a similar way, where also (20) and (21) have to be used.

Let us discuss the operations $[\ ]^i$ and $\{\ \}^i$ defined in (A.2), (A.3), (A.5), (A.6), (A.8), (A.9), and analogous equations. As an example we chose (A.3) and form by

[71] This argument only holds, of course, if the factors are not too singular at equal times. On the basis of the conjecture of Sec. 5, concerning the possibility of multiplying (48) with the step function $\theta(x-y)$, it can be shown that the argument of the text is correct.

linear combination

$$\langle R_{x,u}R_{z,y}\rangle_c=\langle(R_{x,\bar{1}}R_{\bar{2},y})^i\rangle\langle R_{1,u}R_{z,2}\rangle \quad (A.13)$$

and

$$\langle R_{z,y}R_{x,u}\rangle_c=\langle(R_{\bar{2},y}R_{x,\bar{1}})^i\rangle\langle R_{z,2}R_{1,u}\rangle,$$

whereof we need only consider the first relation.

From (39) and (41) we have

$$\langle R_{x,u}'\rangle=\langle R_{x,\bar{1}}{}^{is}\rangle\langle R_{1,u}\rangle\equiv AM$$

and

$$\langle R_{z,y}'\rangle=\langle R_{\bar{2},y}{}^{is}\rangle\langle R_{z,2}\rangle\equiv A'M'.$$

By keeping in mind (43), which was a consequence of (14), we rewrite the lhs of (A.13) symbolically as

$$\langle R_{x,u}R_{z,y}\rangle_c=(e^{(\alpha+\mu)(\alpha'+\mu')}-1)AMA'M',$$

where the small greek letters indicate differentiations of the capital symbols, integrations as in (43) being understood, and c means "connected" as in (A.3b). By rearranging the rhs we obtain

$$\begin{aligned}\langle R_{x,u}R_{z,y}\rangle_c&\\ &=(e^{\alpha\alpha'}-1)AA'\cdot e^{\mu\mu'}MM'\\ &\quad+[e^{\alpha\alpha'}(e^{\alpha\mu'}-1)(e^{\alpha'\mu}-1)+(e^{\alpha\alpha'}-1)(e^{\alpha\mu'}-1)\\ &\quad+(e^{\alpha\alpha'}-1)(e^{\alpha'\mu}-1)]AA'e^{\mu\mu'}MM'\\ &\quad+AA'(e^{\mu\mu'}-1)MM'+[A(e^{\alpha'\mu}-1)A'\\ &\qquad+A'(e^{\alpha\mu'}-1)A]e^{\mu\mu'}MM'. \quad (A.14)\end{aligned}$$

The first term is the first contribution to the rhs of (A.13), namely when both factors in $\langle(R_{x,\bar{1}}R_{2,y})^i\rangle$ are one-particle irreducible. The second term involves "crossing" and necessitates a further splitting of M, or M', or both:

$$M\to BM,\quad M'\to B'M',\quad \mu\to\beta+\mu,\quad \mu'\to\beta'+\mu'.$$

The factor $e^{\mu\mu'}MM'$ always remains and gives the factor $\langle R_{1,u}R_{z,2}\rangle$ in (A.13). There are terms that upon these new splittings do not involve "crossing differentiations" of M or M', and thus immediately contribute to $\langle(R_{x,\bar{1}}R_{z,\bar{2}})^i\rangle$. The terms that involve crossings are treated in the same way in the next step. The two remaining terms in (A.14) produce the one-particle reducibilities at one line, or at both lines, respectively, and are furthermore treated as before. Especially, the penultimate term has, apart from the factor AA', the same structure as we started from.

We thus see that $\langle R_{x,\bar{1}}R_{z,\bar{2}})^i\rangle$ never gets a two-particle reducible contribution, and that the factor is always $\langle R_{1,u}R_{z,2}\rangle$. One can also show that both end lines become $1+A+AB+ABC+\cdots$ and $1+A'+A'B'+A'B'C'+\cdots$, respectively. Not only these expansions break off in any finite order of J, but also the entire expansion of $\langle(R_{x,\bar{1}}R_{z,\bar{2}})^i\rangle$ for any finite momentum transferred, as was remarked in Sec. 3.

Still some more summations can be carried out. On using the formula

$$\begin{aligned}K_{1\cdots N}=&\sum_{\text{perm}}\sum_{\text{part}}(l!m!n!\cdots)^{-1}\\ &\cdot(1+K)K_{1\cdots l}{}^i(1+K)K_{(l+1)\cdots(l+m)}{}^i(1+K)\\ &\cdot K_{(l+m+1)\cdots(l+m+n)}{}^i(1+K)\cdots K_{\cdots N}{}^i(1+K)\end{aligned}$$

derivable from $(1+K)(1-K^i)=1$, where the indices mean functional derivatives, the partitions are those that give $N=l+m+n+\cdots$, with l, m, $n\cdots$ natural numbers, and the permutations are the $N!$ of the indices, one can show that $\langle(R_{\bar{x},\bar{1}},R_{\bar{2},\bar{y}})^i\rangle$ has the structure shown in Fig. 10 as explained in Sec. 3. The difference between the expansion obtained before and the final one just discussed is that in the latter all alined undifferentiated one-particle irreducible parts on the two chains have been summed up. We omit the strictly elementary, but tedious inductive proofs of these statements.

All other irreducible brackets, including those involving (R_3R_4), can be similarly obtained in an explicit form. This way it is also found that, e.g., $\langle[R_x,\tilde{R}_{\bar{2},\bar{1}y}{}^i]^i\rangle$, as defined similarly to (A.6), and $\langle[R_{\bar{x},\bar{y}u}{}^i,R_z]^i\rangle$, as defined by (A.2), become identical upon renaming the indices.

We have here obtained $\langle(R_{x,\bar{u}}R_{\bar{z},y})^i\rangle$, etc. by explicit construction. However, this does not necessarily mean that the solutions of (A.2), (A.3) are unique. If they are so, it will be possible to write them in a form that is analogous to (75), due to the nearly identical structure of (A.2), (A.3) with (60) etc. From such a form, together with the similar formulas that are then derivable for the other irreducible brackets, it can be proved that the sum of the brackets on the rhs of (80) has the same retardedness properties as the irreducible functionals have as was mentioned in Sec. 3.

APPENDIX B

One-Particle Propagator with nonCDD Zeros (Section 5)

Assume $f(z)$ to have nonCDD zeros. These will be zeros at points z_ν, $\bar{z}_\nu$, $\mathrm{Im}z_\nu>0$, $\nu=1\cdots N$, and zeros on the various parts of the real axis. Those real zeros where the real part has positive slope were classified as CDD zeros, so the nonCDD zeros will give negative slope. Both types of zeros can coincide to give zero slope but will, in general, lie apart. We count every zero as often as its multiplicity requires. The real nonCDD zeros will be at x_μ, $\mu=1\cdots M$. We define

$$f(z)=f_r(z)\prod_{\nu=1}^{N}\frac{z-z_\nu}{m^2-z_\nu}\frac{z-\bar{z}_\nu}{m^2-\bar{z}_\nu}\times\prod_{\mu=1}^{M}\left(\frac{z-x_\mu}{m^2-x_\mu}\right)^2\equiv f_r(z)P(z), \quad (B.1)$$

where N and M can be assumed to be infinite[72] but will actually turn out to be finite since at most a polynomial increase of $f(z)$ in infinity is permitted. $f_r(z)$ has only CDD zeros and at the x_μ poles with negative residuum. From (97) and (98) we obtain

$$\mathrm{Im}(-f_r(z)^{-1})\,|_{z=x+0i}=\pi\tilde{\Pi}(x)P(x). \qquad \text{(B.2)}$$

$-f_r(z)^{-1}$ is analytic in the upper z half plane and has, because of $P(x)\geq 0$, nonnegative imaginary part (including possibly delta functions with positive coefficients) along the real axis. A theorem on such functions[73] says that $\mathrm{Im}(-f_r(z)^{-1})$ either is positive in the upper half plane or goes at least linearly to $-\infty$ in some direction. One easily proves that this leads to zeros of $-f_r(z)^{-1}$ excluded by our construction of that function. Therefore the former statement holds and allows to use the representation[74]

$$-f_r(-z)^{-1}=A+Bz+\int_{-\infty}^{+\infty}\frac{1+zt}{t-z}d\sigma(t)$$

with A real, B real nonnegative, and $\sigma(t)$ a real nondecreasing measure. The condition $f_r(m^2)^{-1}=0$ allows to rewrite this as

$$-f_r(z)^{-1}=(z-m^2)B+(z-m^2)\int_{-\infty}^{+\infty}\frac{(1+t^2)d\sigma(t)}{(t-z)(t-m^2)}$$

or, with the help of (B.2),

$$-f_r(z)^{-1}=(z-m^2)B+(z-m^2)\int_{4m^2}^{\infty}\frac{\tilde{\Pi}(t)P(t)}{(t-z)(t-m^2)}dt+(z-m^2)\sum\frac{C_\lambda}{(x_\lambda-z)(x_\lambda-m^2)}, \qquad \text{(B.3)}$$

where $C_\lambda>0$ and x_λ are CDD zeros. The condition $(m^2-z)f_r(z)\,|_{z=m^2}=1$ gives

$$B+\int_{4m^2}^{\infty}\frac{\tilde{\Pi}(t)P(t)}{(t-m^2)^2}dt+\sum\frac{C_\lambda}{(x_\lambda-m^2)^2}=1. \qquad \text{(B.4)}$$

Equations (B.3) and (B.4) give (102) and (103) if nonCDD zeros are absent, i.e., $P(t)\equiv 1$. The behavior of $f(z)$ in infinity is

$$f(z)\to P(z)\cdot(m^2-z)^{-1}\cdot B^{-1} \quad \text{if} \quad B\neq 0,$$

and if $B=0$

$$f(z)\to P(z)\left[\int_{4m^2}^{\infty}\frac{\tilde{\Pi}(t)P(t)dt}{(t-m^2)}+\sum\frac{C_\lambda}{x_2-m^2}\right]^{-1}$$

if the sum and integral exist, or

$$f(z)\to P(z)\left[(m^2-z)\int_{4m^2}^{\infty}\frac{\tilde{\Pi}(t)P(t)dt}{(t-m^2)(t-z)}+(m^2-z)\sum\frac{C_\lambda}{(x_\lambda-2)(x_\lambda-m^2)}\right]^{-1}$$

otherwise, which will be $P(z)$ times a factor that goes to zero not as strongly as z^{-1}. This shows the way in which the behavior of $f(z)$ in infinity and the number of nonCDD zeros are strictly correlated.[75]

If $I>1$ in (105), but $\tilde{\Pi}(t)$, considered as primary quantity, vanishes so strongly in infinity that integrals as in (B.4) converge, it might be possible to satisfy (B.4) by choosing zeros of $P(t)$ in the region where $\tilde{\Pi}(t)$ is not small. In this case a subtracted form of $f(z)$ is defined by (B.1) and (B.3). If, however, $I>1$ and $\tilde{\Pi}(t)$ is not $0(t^{-1})$, no such possibility exists.

If $\tilde{\Pi}(t)$ is considered given, $f_r(z)$ will only have CDD zeros at freely chosen points, and the nonCDD zeros determined by $P(z)$ can be chosen real and positive.

[72] In this case the convergence of the products follows from the at most exponential growth of $f(z)$ in infinity, its reality for real z, and properties of Blaschke products, see, e.g., R. Nevanlinna, *Eindeutige Analytische Funktionen* (Springer-Verlag, Berlin, Germany, 1953), Chap. VII.

[73] This is an adaption of the Phragmen-Lindelöf theorem, see footnote 72, p. 44.

[74] See, e.g., J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, New York, 1943), p. 23.

[75] This was recently shown for the absence of nonCDD zeros by S. Aramaki, Progr. Theoret. Phys. **22**, 485 (1959).

On the Analytic Properties of Partial Wave Amplitudes in Yukawa Potential Scattering

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A new proof is given of the dispersion relation for the lth partial wave amplitude when the potential is of the Yukawa form or (by obvious extension) a suitable linear combination of such forms. The requisite analyticity properties are obtained by rewriting the integral equation for the quantity $f_l(k,r)$, which is related to the l-wave amplitude, as a Volterra equation on a finite interval in which the contribution from the asymptotic part of the integral is absorbed into the inhomogeneous term. The Born series for the inhomogeneous term is analytically continued termwise into the cut complex-wave-number plane and the uniform convergence of the series is then established utilizing approximations which apply in the asymptotic region. The properties of $f_l(k,r)$ then follow from a well-known theorem on Volterra equations.

I. INTRODUCTION

IN a preceding paper[1] one of the authors presented a derivation of the Mandelstam representation for Yukawa potential scattering. In establishing the requisite analyticity character of the scattering amplitude for infinite complex wave number, it was necessary to proceed via an investigation of the behavior of the partial wave projections. This investigation was conducted rigorously only for the $l=0$ wave, but an analysis for higher l has been given by Martin.[2,3] While previously the knowledge of partial wave properties assumed an auxiliary character, examination of the field theoretic applications of the Mandelstam representation[4] suggests that it be regarded as of primary significance. In the present note we shall present a new derivation of the lth wave dispersion relation for Yukawa potential scattering which provides considerable clarification of the mathematical difficulties involved. In particular it will be shown that the required analyticity properties depend only on the behavior of solutions of the radial equations in regions where the complexities associated with $l>0$ disappear.

II. STATEMENT OF THE PROBLEM

The radial Schrödinger equation for the lth partial wave $\phi_l(k,r)$ corresponding to a potential $V(r)$ is

$$\{d^2/dr^2+k^2-V(r)-l(l+1)/r^2\}\phi_l(k,r)=0, \quad (1)$$

where $\hbar=2m=1$ and k is the wave number. $\phi_l(k,r)$ obeys the boundary condition $\phi_l(k,0)=0$, but may be conveniently expressed in terms of a solution $f_l(k,r)$ satisfying the asymptotic boundary condition

$$f_l(k,r)\rightarrow \exp[-i(kr-\tfrac{1}{2}l\pi)], \; r\rightarrow\infty. \quad (2)$$

In fact,

$$\phi_l(k,r)=(-i^l/2ik)(2l+1)f_l^{-1}(-k) \times\{f_l(-k)f_l(k,r)-(-)^l f_l(k)f_l(-k,r)\}, \quad (3)$$

where

$$f_l(k)\equiv\lim_{r\rightarrow 0}\frac{(2kr)^l}{(l,l)}f_l(k,r), \quad (l,m)\equiv\frac{(l+m)!}{(l-m)!m!}. \quad (4)$$

One then obtains for the asymptotic form of $\phi_l(k,r)$

$$\phi_l(k,r)\overset{r\rightarrow\infty}{\longrightarrow}\frac{i^l}{k}(2l+1)\exp[i\delta_l(k)]\sin[kr-\tfrac{1}{2}l\pi+\delta_l(k)], \quad (5)$$

with

$$\exp[2i\delta_l(k)]=f_l(k)/f_l(-k). \quad (6)$$

In the present study we shall investigate the analytic properties of $f_l(k)$ for the Yukawa potential

$$V(r)=\lambda e^{-\mu r}/r. \quad (7)$$

This will then enable us to write a dispersion relation for the l-wave scattering amplitude

$$A_l(k)=(2ik)^{-1}[\exp[2i\delta_l(k)]-1]. \quad (8)$$

III. ANALYTIC PROPERTIES OF $f_l(k)$

In this section it will be proved that (A) $f_l(k)$ is an analytic function of k in the entire k plane excluding a branch cut (denoted Ω) which consists of the half-line $k=i\mu/2\rightarrow i\infty$.

Statement (A) as restricted to $\mathrm{Im}k<0$ is well known for a very wide class of potentials including the Yukawa potential. In fact when $V(r)$ satisfies

$$\int_0^\infty r|V(r)|dr<\infty, \quad \int_0^\infty r^2|V(r)|dr<\infty,$$

it has been shown[5] that $f_l(k)$ is analytic in $\mathrm{Im}k<0$ and

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[1] A. Klein, J. Math. Phys. 1, 41 (1960).
[2] A. Martin, Nuovo cimento 14 (403) 1959.
[3] A. Martin, Nuovo cimento (to be published). Related work has been carried out by R. E. Peierls (preprint).
[4] G. Chew and S. Mandelstam, Phys. Rev. (to be published).
[5] R. Jost and R. Newton, Nuovo cimento 1, 590 (1955). (This reference contains a plethora of detail about analyticity properties in $\mathrm{Im}k\leqslant 0$ and also references to previous papers on the subject.)

approaches unity as $|k| \to \infty$. The zeros of $f_l(k)$ are the eigenvalues of (1) and may occur only for $k=-iK$ with $K>0$. Since neither $k=0$ or $k=-i\infty$ can be an accumulation point of zeros of $f_l(k)$,[5] the analyticity of $f_l(k)$ in $\mathrm{Im}k<0$ implies that the number of eigenvalues is finite.

It is noteworthy that only the properties of $f_l(k)$ in $\mathrm{Im}k\leqslant 0$ are needed to establish the Levinson theorem and the Levitan-Gel'fand formalism[5] for the construction of potentials from phase shifts and bound—state data. On the other hand, the derivation of a useful dispersion relation for $A_l(k)$ will require an excursion into the murkier reaches of the upper half—k plane, where the assumption of Yukawa-like behavior of the potential becomes crucial.

It is convenient to introduce the function $h_l(\rho)$ related to the spherical Hankel function of the second kind

$$h_l(\rho)=-i\rho h_l^{(2)}(\rho)=(l,l)/(2\rho)^l\kappa_l(\rho)e^{-i\rho}, \tag{9a}$$

where $\kappa_l(\rho)$ are polynomials of degree l in ρ:

$$\kappa_l(\rho)=\sum_{m=0}^{l}\frac{(l,l-m)}{(l,l)}(2i\rho)^m; \tag{9b}$$

and to define the function

$$\mathfrak{F}_l(k,r)=[(2kr)^l/(l,l)]e^{ikr}f_l(k,r), \tag{10}$$

so that

$$\mathfrak{F}_l(k,r)\to f_l(k) \text{ as } r\to 0$$
$$\mathfrak{F}_l(k,r)\to \kappa_l(kr) \text{ as } r\to\infty. \tag{11}$$

Equations (1), (2), and (10) imply

$$\mathfrak{F}_l(k,r)=\kappa_l(kr)+\int_r^\infty \mathcal{G}_l^{(0)}(k;r,r')V(r')\mathfrak{F}_l(k,r')dr', \tag{12}$$

where

$$\mathcal{G}_l^{(0)}(k;r,r')=\begin{cases} 0: & r'\leqslant r \\ \dfrac{(-)^l}{2ik}\left(\dfrac{r}{r'}\right)^l\exp[-ik(r'-r)] & \\ \quad\times[h_l(kr)h_l(-kr') & \\ \quad -h_l(-kr)h_l(kr')]: & r'\geqslant r. \end{cases} \tag{13}$$

Examination of (12) and (13) reveals that convergence difficulties are encountered for $\mathrm{Im}k\geqslant(\mu/2)$ because of the divergent factor $\exp[-(\mu+2ik)(r'-r)]$ as $|k|(r'-r)\to\infty$, i.e., as $|k|r'\to\infty$ for finite r. On the other hand, the form of $\mathcal{G}_l^{(0)}(k;r,r')$ may be considerably simplified for $|k|r'\to\infty$. This suggests that we rewrite (12) in the form

$$\mathfrak{F}_l(k,r)=\xi_l^{(R)}(k,r)+\int_r^R \mathcal{G}_l^{(0)}(k;r,r')V(r')\mathfrak{F}_l(k,r')dr', \tag{14}$$

where

$$\xi_l^{(R)}(k,r)=\kappa_l(kr)+\int_R^\infty \mathcal{G}_l^{(0)}(k;r,r')V(r')\mathfrak{F}_l(k,r')dr', \tag{15}$$

and $R>r$ is at our disposal. Since (14) is a Volterra equation on a finite interval, the Neumann series solution obtained from (14) satisfies[6]

$$|\mathfrak{F}_l(k,r)|\leqslant|\max_{r\leq r'\leq R}\xi_l^{(R)}(k,r')| \times\exp|\max_{r\leq r'\leq R}\mathcal{G}_l^{(0)}(k;r,r')V(r')|(R-r). \tag{16}$$

Since $\mathcal{G}_l^{(0)}(k;r,r')$ vanishes like $r'-r$ as $r'\to r$ and is analytic in k for finite $|k|$, it follows that $|\mathfrak{F}_l(k,r)|$ is bounded in k for k in some finite region K and $0\leqslant r\leqslant R$, provided that $|\xi_l^{(R)}(k,r)|$ is likewise bounded. If in fact $\xi_l^{(R)}(k,r)$ were analytic in k for a closed region K and $0\leqslant r\leqslant R$, the Neumann series for (14) would be term-wise analytic and uniformly convergent on the contour of K thus implying the analyticity of $\mathfrak{F}_l(k,r)$ for $k\epsilon K$.

In Sec. IV we shall establish the following:

(B) Given $|k_0|>0$, there exists $C\gg 1$ such that for $R=C/|k_0|$, $\xi_l^{(R)}(k,r)$ can be analytically continued from the representation (15) on the real k axis into the entire finite k plane outside the circle $|k|=|k_0|$ exclusive of the cut Ω.

The analytic continuations of $\mathfrak{F}_l(k,r)$ constructed for various R say $C/|k_0|$ and $C/|k_1|$ clearly coincide for real k with $|k|\geqslant\max(|k_0|,|k_1|)$, and hence throughout the common region of analyticity. Thus for all k with $|k|\geqslant|k_0|$:

$$\mathfrak{F}_l(k,0)=\xi_l^{(C/|k_0|)}(k,0)+\int_0^{C/|k_0|}\mathcal{G}_l^{(0)}(k;0,r')V(r')\mathfrak{F}_l(k,r')dr'$$
$$=\xi_l^{C/|k|}(k,0)+\int_0^{C/|k|}\mathcal{G}_l^{(0)}(k;0,r')V(r')\mathfrak{F}_l(k,r')dr'. \tag{17}$$

Hence the behavior as $|k|\to\infty$ of the continuation of $\mathfrak{F}_l(k,0)$ constructed for a fixed $R=C/|k_0|$ may be obtained from an analysis of

$$\lim_{|k|\to\infty}\xi_l^{C/|k|}(k,0).$$

In Sec. IV we shall prove

$$\textbf{(C)}\quad \lim_{\substack{|k|\to\infty \\ \text{outside } \Omega}}|\xi_l^{(C/|k|)}(k,0)-1|=o(\lambda|\ln k|/|k|).$$

[6] F. Riesz and B. Sz. Nagy, *Functional Analysis* (F. Ungar, New York, 1956), p. 147.

Then from the second line of (17), the Born series for $\mathfrak{F}_l(k,0)$ approaches its zeroeth term, i.e.,

$$\lim_{\substack{|k|\to\infty \\ \text{outside } \Omega}} |\mathfrak{F}_l(k,0)-1| = 0(\lambda|\ln k|/|k|). \tag{18}$$

Thus from (9) and (11)

$$\lim_{\substack{|k|\to\infty \\ \text{outside } \Omega}} f_l(k) = 1+0(\lambda|\ln k|/|k|). \tag{19}$$

We have therefore reduced the proof of (**A**) to a proof of (**B**) and (**C**) which we shall next undertake.

IV. PROOF OF STATEMENTS (B) AND (C)

We shall investigate the Born series for $\xi_l^{(R)}(k,r)$ obtained by integration of (15) with (12). Each term consists of factors of the form $\int_R^\infty \mathcal{G}_l^{(0)}(k;r,r')V(r')\times\kappa_l(kr')dr'$ with $R=r$ in all but the first factor. Note that all variables of integration exceed R. After some rearrangement we may write

$$\int_R^\infty \mathcal{G}_l^{(0)}(k;r,r')V(r')\kappa_l(kr')dr'$$

$$= e^{-2ik(R-r)}\frac{\kappa_l[-k(d/d\mu)]}{\kappa_l(-kR)}\Big\{\Lambda_0(k,r,R)$$

$$\cdot R\int_R^\infty \left(\frac{r'}{R}\right)^{-2l}\kappa_l(-kr')\frac{\exp(-\mu r')}{r'}dr'$$

$$+\lambda\kappa_l(-kr)A_l(\mu,k,R)\Big\}, \tag{20}$$

where we have used

$$\kappa_l(kr)e^{-\mu r} = \kappa_l(-kd/d\mu)e^{-\mu r},$$

and defined

$$\Lambda_0(k,r,R) \equiv e^{ik(R-r)}[(-)^l/2ikR](r/R)^l \times[h_l(kr)h_l(-kR)-h_l(-kr)h_l(kR)], \tag{21}$$

and

$$A_l(\mu,k,R) \equiv \frac{(-1)^l}{2ik}\int_R^\infty \exp -ik(r'-R)\left(\frac{R}{r'}\right)^l \times[h_l(kR)h_l(-kr')-h_l(-kR)h_l(kr')] \times\exp(-\mu r')\frac{dr'}{r'}. \tag{22}$$

The form (20) is especially convenient for analytic continuation. It is shown in Appendix I that for real k,

$$A_l(\mu,k,R) = \int_\mu^\infty \frac{e^{-\alpha R}d\alpha}{\alpha(\alpha+2ik)}\left\{\frac{\mu(\mu+2ik)}{\alpha(\alpha+2ik)}\right\}^l. \tag{23}$$

One observes that $A_l(\mu,k,R)$ is analytic in k in the finite k plane exclusive of the branch-cut Ω. The first integral in (20) is an entire function of k and is conveniently rewritten

$$R\int_R^\infty \left(\frac{r'}{R}\right)^{-2l}\kappa_l(-kr')\frac{\lambda\exp(-\mu r')}{r'}dr' = R\int_\mu^\infty \left(\frac{\mu}{\alpha}\right)^{2l}\kappa_l\left(-\frac{k}{\mu}\alpha R\right)\frac{e^{-\alpha R}}{\alpha}d\alpha. \tag{24}$$

Thus

$$\int_R^\infty \mathcal{G}_l^{(0)}(k,r,r')V(r')\kappa_l(kr')dr' = \lambda e^{-2ik(R-r)}\frac{\kappa_l[-k(d/d\mu)]}{\kappa_l(-kR)} \times\int_\mu^\infty \Lambda_l(r,R,k,\mu,\alpha)e^{-\alpha R}d\alpha, \tag{25}$$

where

$$\Lambda_l(r,R,k,\mu,\alpha) = \frac{1}{\alpha}\left(\frac{\mu}{\alpha}\right)^l\left[\Lambda_0(k,r,R)\kappa_l(-k\alpha R/\mu)R\left(\frac{\mu}{\alpha}\right)^l + \kappa_l(-kr)(\mu+2ik)^l/(\alpha+2ik)^{l+1}\right]. \tag{26}$$

For $|k|R\gg 1$, $+\mathrm{Im}k>0$ we obtain from (21) the useful approximation

$$\Lambda_l(r,R,k,\mu,\alpha) \cong \frac{1}{\alpha}\left(\frac{\mu}{\alpha}\right)^l\kappa_l(-kr)\left[-\frac{1}{2ik}+\frac{(\mu+2ik)^l}{(\alpha+2ik)^{l+1}}\right]. \tag{27}$$

The analytic continuation of (20) by means of (23) must now be applied to each term of the Born series for $\xi_l^{(R)}(k,r)$. The second Born approximation for example is

$$\lambda^2\frac{\exp[-2ik(R-r)]}{\kappa_l(-kR)}\kappa_l(-kd/d\mu_1)_{\mu_1=\mu} \times\int_{\mu_1}^\infty \frac{\exp(-\alpha R)d\alpha}{\alpha(\alpha+2ik)}\left[\frac{\mu_1(\mu_1+2ik)}{\alpha(\alpha+2ik)}\right]^l \times\int_\mu^\infty \Lambda_l(r,R,k,\mu+\alpha,\beta+\alpha)e^{-\beta R}d\beta. \tag{28}$$

The series becomes

$$\xi_l^{(R)}(k,r) = \kappa_l(kr)+\frac{\exp[-2ik(R-r)]}{\kappa_l(-kR)} \times\sum_{n=0}^\infty \lambda^{n+1}B^{(n)}(\mu,k,r,R), \tag{29}$$

where

$$B_l^{(n)}(\mu,k,r,R)$$

$$=\kappa_l[-k(d/d\mu_1)]_{\mu_j=\mu}\prod_{j=1}^{n}$$

$$\times\int_{\mu_j}^{\infty}\frac{(\mu_j+\sum_{\nu=1}^{j-1}\alpha_\nu)^l(\mu_j+2ik+\sum_{\nu=1}^{j-1}\alpha_\nu)^l e^{-\alpha_j R}d\alpha_j}{(\sum_{\nu=1}^{j}\alpha_\nu)^{l+1}(2ik+\sum_{\nu=1}^{j}\alpha_\nu)^{l+1}}$$

$$\times\int_{\mu}^{\infty}\Lambda_l(r,R,k,\mu+\sum_{\nu=1}^{n}\alpha_\nu,\alpha+\sum_{\nu=1}^{n}\alpha_\nu)e^{-\alpha R}d\alpha. \quad (30)$$

where

$$\mu_j=\mu+\delta_{j1}(\mu_1-\mu)$$

To establish the convergence of (29) for finite $|k|$ it suffices to prove convergence for the expression obtained from (29) and (30) by the replacement

$$\sum_{n=0}^{\infty}\prod_{j=1}^{n}\to\sum_{n=N_0}^{\infty}\prod_{j=N_0}^{\infty};\quad N_0=\left[\frac{2|\mathrm{Im}k|}{\mu}\right]+1,$$

$[a]$=smallest integer $>a$. With this replacement it is clear that since

$$\sum_{\nu=1}^{j}\alpha_\nu\geqslant j\mu\geqslant 2\,\mathrm{Im}k\quad\text{for all } j\geqslant N_0,$$

then

$$\left|\frac{(\mu_j+\sum_{\nu=1}^{j-1}\alpha_\nu)}{(\sum_{\nu=1}^{j}\alpha_\nu)}\frac{(\mu_j+2ik+\sum_{\nu=1}^{j-1}\alpha_\nu)}{(2ik+\sum_{\nu=1}^{j}\alpha_\nu)}\right|\geqslant 1. \quad (31)$$

Now we note that if R is chosen such that μR is sufficiently large, the principal contributions to the integrals over α and $\alpha_j(j=N_0\cdots,n)$ in (30) arise from $\alpha_\nu\cong\mu_\nu$, $\nu=1,\cdots,j$. Furthermore, the principal contributions to the derivative $d/d\mu$ arise from the exponential $\exp(-\mu R)$. If we then choose R so large that these approximations and in addition (27) are valid, we obtain

$$|B^{(n\geqslant N_0)}(\mu,k,r,R)|\leqslant\mathrm{const}\prod_{j=N_0}^{n}$$

$$\times\left|\frac{e^{-\mu R}}{(j\mu R)(2ik+j\mu)}\right|\left|\kappa_l(-kr)\frac{e^{-\mu R}}{(n+1)\mu R}\right.$$

$$\left.\times\left(-\frac{1}{2ik}+\frac{1}{2ik+(n+1)\mu}\right)\right|\leqslant C(N_0,\mu,k,r)$$

$$\times[n!(n-N_0)!]^{-1}\left|\frac{1}{\mu^2 R}e^{-\mu R}\right|^n, \quad (32)$$

where $C(N_0,\mu,k,r)$ is bounded for finite r and finite $|k|$ exclusive of Ω. From (32) we may conclude that for finite k outside Ω, $|k|\geqslant|k_0|$, $R=C/|k_0|$ and C sufficiently large that the remarks following (31) are applicable, (29) converges to an analytic function. It must be remarked also that C is to be chosen such that $\kappa_l(-kR)$ has no zeros for $|k|R\geqslant C$. This is of course possible for finite l. The proof of statement (B) is now complete.

In Appendix II it is shown that the product of the left side of (31) for $j=1, 2, \cdots n$ is majorized by a^n, where a is a constant independent of k excluding an arbitrarily small band enclosing Ω. Examination of the series (29) for $R=C/|k|$ then shows that C can be chosen sufficiently large that the remarks following (31) apply. One thus obtains:

$$\lambda^{n+1}|B_l^{(n)}(\mu,k,0,C/|k|)|$$

$$\leqslant|C_l'(\mu,C)|^{n+1}\prod_{j=1}^{n+1}\left|\int_{\mu}^{\infty}\frac{\lambda d\alpha_j}{(\sum_{\nu=1}^{j}\alpha_\nu)(2ik+\sum_{\nu=1}^{j}\alpha_\nu)}\right|, \quad (33)$$

where $C_l'(\mu,C)$ is a bounded function of μ and C. The last factor is precisely that which is encountered for the case $l=0$ and is easily shown to satisfy the inequality for large $|k|$:

$$\prod_{j=1}^{n+1}\left|\int_{\mu}^{\infty}\frac{\lambda d\alpha_j}{(\sum_{\nu=1}^{j}\alpha_\nu)(2ik+\sum_{\nu=1}^{j}\alpha_\nu)}\right|\leqslant\left(\frac{\lambda\ln|k|}{|k|}\right)^{n+1}. \quad (34)$$

Substitution of (33) and (34) into (29) yields

$$\lim_{\substack{|k|\to\infty\\ \text{outside }\Omega}}\xi_l^{(C/|k|)}(k,0)=1+0\left(\frac{\lambda\ln|k|}{|k|}\right), \quad (35)$$

which concludes the proof of Statements (C).

V. CONCLUSIONS

It has now been established that for a Yukawa potential the l-wave scattering amplitude $A_l(k)$ is analytic in the upper half k plane, except for a branch cut on the imaginary k axis extending from $k=i\mu/2$ to $k=i\infty$ and a finite number of poles, also on the imaginary k axis, corresponding to the bound states. The difference between $A_l(k)$ and its first Born approximation $A_l^{(0)}(k)$ may then be shown to have the branch cut from $k=i\mu$ to $k=i\infty$. Application of Cauchy's theorem to $A_l(k)-A_l^{(0)}(k)$ in the variable $s=k^2$ with the contour of Fig. 1 produces the dispersion relation

$$A_l(s^{\frac{1}{2}})-A_l^{(0)}(s^{\frac{1}{2}})$$

$$=\sum_i C_{li}/(s-s_{li})+\frac{1}{\pi}\int_0^{\infty}\frac{\mathrm{Im}A_l(s'^{\frac{1}{2}})}{s'-s}$$

$$+\frac{1}{\pi}\int_{-\infty}^{-\mu^2}\frac{\mathrm{Im}\{A_l(s'^{\frac{1}{2}})-A_l^{(0)}(s'^{\frac{1}{2}})\}}{s'-s}ds', \quad (36)$$

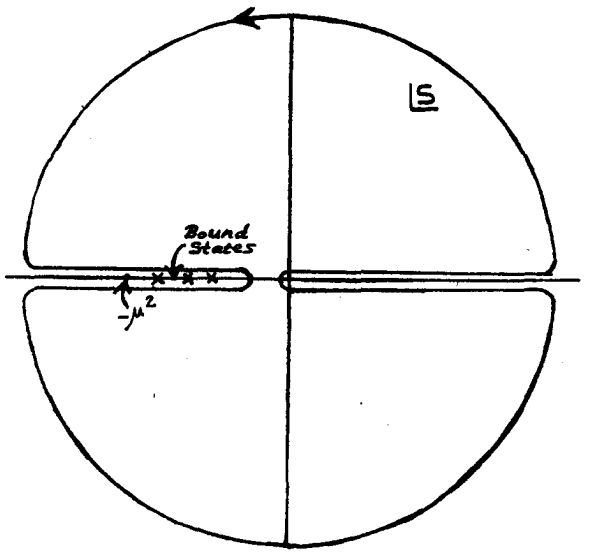

FIG. 1. Contour for Cauchy integral for $A_l(s^{\frac{1}{2}})$.

where

$$A_l^{(0)}(s^{\frac{1}{2}})=(-\lambda/2s)Q_l[(\mu^2+2s)/2s],$$

$Q_l(v)$ are Legendre functions of the second kind

$$Q_0(\nu)=\tfrac{1}{2}\ln(\nu+1/\nu-1)$$
$$(l+1)Q_{l+1}(\nu)=(2l+1)\nu Q_l(\nu)-lQ_{l-1}(\nu)$$

and C_i are residues at the bound state energies s_{li}.

APPENDIX I

$$A_l(k,\mu,r)\equiv\frac{1}{2ik}\int_r^\infty\left(\frac{r}{r'}\right)^l\sum_{m,n=0}^{l}\frac{(l,m)(l,n)}{(2ikr)^m(2ikr')^n}$$
$$\times\{(-1)^n-(-1)^m\exp[-2ik(r'-r)]\}$$
$$\times\frac{\exp(-\mu r')}{r'dr'}. \quad (I.1)$$

If $2\,\mathrm{Im}k<\mu$, successive integrations by parts yield the relation

$$\int_r^\infty\frac{r^m}{r'^n}\exp[-2ik(r'-r)-\mu r']\frac{dr'}{r'}$$
$$=\frac{(-1)^n}{n!}(\mu+2ik)^n\left\{(-1)^m m!\int_\mu^\infty\frac{e^{-\alpha r}d\alpha}{(\alpha+2ik)^{m+1}}\right.$$
$$+\sum_{\lambda=1+\min(n,m)}^{\max(n,m)}(-1)^\lambda(\mu+2ik)^{-\lambda}$$
$$\left.\times(\lambda-1)!e^{-\mu r}r^{m-\lambda}\right\}. \quad (I.2)$$

If we introduce (I.2) into (I.1) and simplify, we obtain from those terms arising from the first term of (I.2)

$$\int_\mu^\infty\frac{e^{-\alpha r}d\alpha}{\alpha(\alpha+2ik)}\left\{\frac{\mu(\mu+2ik)}{\alpha(\alpha+2ik)}\right\}^l\sum_{m=0}^{l}\binom{l+m}{m}$$
$$\times\{y^m(1-y)^{l+1}+y^{l+1}(1-y)^n\}, \quad (I.3)$$

where $y=(-\alpha/2ik)$. The summation in (I.3) is unity for arbitrary y. The contributions to (I.1) from the second term of (I.2) yield a polynomial

$$\sum_{\nu=1}^{2l}\sum_{j=0}^{2l-\nu}C_{\nu j}r^\nu(\mu/2ik)^j,$$

in which the coefficients are various sums of products of binomial coefficients all of which are readily proven to vanish. Thus

$$A_l(k,\mu,r)=\int_\mu^\infty\frac{e^{-\alpha r}d\alpha}{\alpha(\alpha+2ik)}\left\{\frac{\mu(\mu+2ik)}{\alpha(\alpha+2ik)}\right\}^l. \quad (I.4)$$

APPENDIX II

The proof of the following inequality is required in the text:

$$\left|\prod_{j=1}^{n}\left(\frac{\mu+\sum_{\nu=1}^{j-1}\alpha_\nu}{\sum_{\nu=1}^{j}\alpha_\nu}\right)\left(\frac{\mu+2ik+\sum_{\nu=1}^{j-1}\alpha_\nu}{2ik+\sum_{\nu=1}^{j}\alpha_\nu}\right)\right|\leqslant a^n, \quad (II.1)$$

for arbitrary k excluding Ω, where a is a constant independent of k. For $2\,\mathrm{Im}k\leqslant\mu$ the left side is majorized by unity (obtained by setting $\alpha_j=\mu$ for all j). Now suppose $2\,\mathrm{Im}k\geqslant\mu$. The left side of (II.1) can be written

$$\left|\frac{\mu(\mu+2ik)}{\zeta_n(\zeta_n+2ik)}\right|\left|\prod_{j=1}^{n-1}\frac{(\mu+\zeta_j)(\mu+2ik+\zeta_j)}{\zeta_j(2ik+\zeta_j)}\right|, \quad (II.2)$$

where

$$\zeta_j=\sum_{\nu=1}^{j}\alpha_j\geqslant j\mu.$$

Clearly

$$\left|\frac{\mu+\zeta_j}{\zeta_j}\right|\leqslant 2.$$

The maximum of

$$\left|\frac{\mu+2ik+\zeta_j}{2ik+\zeta_j}\right|$$

occurs for

$$\zeta_j-2\,\mathrm{Im}k=\frac{[-\mu+\{\mu^2+16(\mathrm{Re}k)^2\}^{\frac{1}{2}}]}{2},$$

and applying $(a^2+b^2)^{\frac{1}{2}} \leqslant |a|+|b|$ one obtains

$$\left|\frac{\mu+2ik+\zeta_j}{2ik+\zeta_j}\right| \leqslant 2\left(1+\frac{\mu}{4(\mathrm{Re}k)}\right)<\infty$$

provided that $|\mathrm{Re}k| \geqslant \epsilon>0$. The maxima of $|\mu(\mu+2ik)/\zeta_n(\zeta_n+2ik)|$ occur when $\zeta_n=\mu$ and

$$\zeta_n=\frac{3\,\mathrm{Im}k+\{(\mathrm{Im}k)^2-8(\mathrm{Re}k)^2\}^{\frac{1}{2}}}{2}.$$

In the first case the value is unity. In the second case suppose first that $\mathrm{Im}k \leqslant N|\mathrm{Re}k|$, where $N \gg 2\sqrt{2}$. Then

$$\left|\frac{\mu(\mu+2ik)}{\zeta_n(\zeta_n+2ik)}\right| \leqslant \sim N/2.$$

On the other hand, if $\mathrm{Im}k \geqslant N|\mathrm{Re}k|$ then the second maximum occurs at $\zeta_n \cong 2\,\mathrm{Im}k$, where its value is majorized by

$$\mu/2|\mathrm{Re}k|<\infty \quad \text{if} \quad |\mathrm{Re}k| \geqslant \epsilon>0.$$

Thus taking $a=\max(N/2,\ 4(1+\mu/4|\mathrm{Re}k|)$ (II.1) follows.

Invariant Imbedding and Mathematical Physics. I. Particle Processes

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With the use of invariance principles in a systematic fashion, we shall derive not only new analytic formulations of the classical particle processes, those of transport theory, radiative transfer, random walk, multiple scattering, and diffusion theory, but, in addition, new computational algorithms which seem well fitted to the capabilities of digital computers. Whereas the usual methods reduce problems to the solution of systems of linear equations, we shall try to reduce problems to the iteration of nonlinear transformations.

Although we have analogous formulations of wave processes, we shall reserve for a second paper in this series a detailed and extensive treatment of this part of mathematical physics.

CONTENTS

I. INTRODUCTION

THE classical equations of the processes of mathematical physics can be put in the form

$$u_t = T(u), \tag{1}$$

where u is a vector function of a space vector p, restricted to a region R, and the time $u=u(p,t)$. The operator T is in many cases a linear partial differential operator, in some cases a linear integral operator, and if we insist upon realism, a nonlinear operator. The steady-state version is obtained by setting the vector u_t equal to zero.

Since equations of this type usually have an infinite number of solutions, it is necessary to attach some further restrictions in order to single out a particular solution. To do this, we usually assign initial values,

$$u(p,0)=v(p), \quad p \epsilon R, \tag{2}$$

and boundary values

$$u(p,t)=w(p,t), \tag{3}$$

for $p\epsilon B$, the boundary of R.

Problems of this nature have two types of difficulties associated, difficulties which are inseparably intertwined, those of analytic character and those of computational nature. Among the many methods which have been proposed is the theory of semigroups. The guiding ideas were first enunciated by Hadamard, and subsequently were systematically pursued by Hille and Yosida; see Hille and Phillips[1] for a thorough exposition and many references. Classically, the semigroup concept has been exploited in the time domain. Our aim is to show that this basic method can be applied in a much wider area, using other physical variables of significance as semigroup variables.

If we use invariance principles in a systematic fashion, we shall derive not only new analytic formulations of the classical particle processes, those of transport theory, radiative transfer, random walk, multiple scattering, and diffusion theory, but, in addition, new computational algorithms which seem well fitted to the capabilities of digital computers. Whereas the usual methods reduce problems to the solution of systems of linear equations, we shall try to reduce problems to the iteration of nonlinear transformations.

Although we have analogous formulations of wave processes,[2–4] we shall reserve for a second paper in this series a detailed and extensive treatment of this part of mathematical physics.

Our interest in the field of invariance principles was aroused by the elegant and fundamental work of Chandrasekhar in the theory of radiative transfer.[5] His results, in turn, are generalizations of those of Ambarzumian who seems to have been the first to have consciously employed invariance principles in any significant fashion.[6] Since then, in addition to our work, reference to which will be made later in the paper, there have been important contributions by Preisendorfer,[7,8] Ramakrishnan,[9] Redheffer,[10] and Ueno.[11–13] In addition, there are some unpublished results due to T. E. Harris.

Independently, functional equation techniques were introduced into the theory of branching processes, in particular, those arising in cosmic ray cascade theory and biological mutation, by Bellman and Harris,[14,15] and Janossy.[16] Surveys of the many results obtained over the last ten years may be found in Harris[17,18] and Ramakrishnan.[19] Also in the theory of dynamic programming,[20] in connection with the treatment of minimization and maximization problems, we find a use of invariance principles and functional equations which is quite similar in spirit to what we shall find below in the treatment of purely descriptive processes.

In place of beginning with an abstract formulation of particle processes and an abstract presentation of the principles of invariant imbedding, we shall start with a study of a particular process, neutron transport and multiplication. The difference in formulation between the usual approach and that furnished by "invariant imbedding," as we shall call our systematic application of invariance principles, will readily be seen. Nevertheless, as we shall show, both are merely particular instances of a general approach.

Having gone through a spectrum of transport processes, steady-state and time-dependent, energy-independent and energy-dependent, one-dimensional and multi-dimensional, unchanging medium and Stefan-type, we shall abstract the basic ideas of invariant imbedding.

Following this, we shall apply these techniques to the study of random walk and multiple scattering, to the study of radiative transfer and diffusion. Our treatment of these fields will be much briefer since much of what is done in the part devoted to neutron transport can easily be transcribed and applied in these other areas.

In what follows, we shall pursue a purely formal path, leaving aside all questions of existence, uniqueness, and so on. What is interesting, however, is that our approach enables us to handle many of these questions in a much simpler and straightforward way than that furnished by the conventional road.

Although we are in part motivated by a search for feasible computational techniques, we shall actually avoid any discussion of actual numerical techniques. In subsequent papers we shall treat these matters in great detail. Here we shall restrain ourselves to generalities.

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[2] R. Bellman and R. Kalaba, Proc. Natl. Acad. Sci. U. S. 44, 317 (1958).

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The equations of invariant imbedding are related to the variational formulas of Hadamard type, expressing the dependence of the Green's function of a region upon the dimensions of the region.[21]

Finally, let us note that no previous knowledge of the equations of mathematical physics is required. All equations will be derived from first principles, directly from the mathematical model of the physical process.

II. NEUTRON TRANSPORT AND MULTIPLICATION

1. Introduction

Let us begin our journey with the examination of a number of intriguing mathematical problems which arise in the study of various aspects of neutron transport and multiplication. A consideration of some of the many different hypotheses that can be made will give us an opportunity to display the versatility of the theory of invariant imbedding.

Our basic assumption is that a neutron is a point particle which is completely specified at any time by its direction of motion and its energy. These two properties determine its state. As the neutron traverses the medium within which the transport process takes place, it suffers certain changes of state (i.e., changes in energy and direction), as a result of interactions with the medium and with other neutrons. In addition, we have the relatively new and very important phenomenon of fission. Certain interactions can result in an increase in the number of neutrons, the fission process.

The probabilities of these events are measured by "cross sections" or "mean free paths." Occasionally, we shall talk in deterministic terms, and occasionally in stochastic terms, depending upon which is more convenient. The difference is more apparent than real, since the use of expected values in a stochastic model leads to a completely deterministic version based upon fluxes.

Within the framework of a mathematical model constructed along these lines, a model we shall make more precise in the following section, we wish to explain and predict the phenomenon of criticality, and to determine the internal and external fluxes as functions of the spatial dimensions, the time, and other parameters. Problems of this nature are of great complexity from the mathematical side, and thus of even greater fascination, even when greatly simplified physical models are used. When more realistic assumptions are made, the analytic aspects become truly formidable, and the problem of obtaining numerical results much more burdensome.

It is not to be expected that recondite scientific questions will yield readily to any single approach. Rather it is to be expected that with the aid of a battery of methods, each of which chips away at some of the obstacles in our path, we can eventually clear a road which will take us some distance toward our goal.

The classical equations of transport theory can be effectively applied in a number of cases. Approximate methods of various degrees of efficacy and associated results may be found in the book by Davison.[22] Rigorous discussion of these techniques can lead to quite complex analysis; see for example the papers by Lehner and Wing,[23–26] Jorgens,[27] and Pimbley.[28]

A number of questions can be studied by means of the mathematical theory of branching processes. The study of age-independent processes was begun by Harris,[17,18] and Everett and Ulam,[29] independently of each other. Essentially it reduces to the study of the iteration of power series, with probabilistic overtones. The theory of age-dependent branching processes, based upon the systematic usage of functional equations, was begun by Bellman and Harris,[14,15] and independently by Janossy.[16] Detailed expositions with many references will be found in the monograph by Harris,[17] the expository papers by Harris,[18] and Ramakrishnan.[19]

It is natural to construct simplified models in a situation characterized by severe mathematical difficulties and by physical complexity as well. The usual hope is that the exploration of these models will furnish valuable experience and that the understanding of these more transparent models will enable us to penetrate into the more obscure versions. However, as mentioned above, even apparently simple processes give rise to sophisticated analysis.

Furthermore, as we shall discuss repeatedly below, unless the problems are carefully formulated they cannot be resolved in numerical terms in any straightforward fashion. Our objective in the pages that follow is to formulate a variety of transport processes in a way which will permit us to obtain numerical solutions with the aid of digital computers. As is often the case in mathematics and physics, a significant improvement in computational technique requires a new conceptual and analytic approach.

It turns out that in the process of fulfilling one of our goals, numerical solution of problems, we obtain as byproducts a host of interesting and elegant analytic results, together with powerful methods for establishing existence and uniqueness theorems for the associated functional equations and for the classical functional equations of mathematical physics. Many of these equations are quite difficult to treat along conventional lines.

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[23] J. Lehner and G. M. Wing, Commum. Pure and Appl. Math. 8, 217 (1955).

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[25] G. M. Wing, "Transport theory and spectral problems," *Proc. Symposium on Reactor Theory* (American Mathematical Society, Providence, Rhode Island) to be published.

[26] J. Lehner, Commum. Pure Appl. Math. **9**, 487 (1956).

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[29] C. J. Everett and S. Ulam, Los Alamos Scientific Lab., declassified documents LADC-534 (AECD-2164), May 6, 1948; LADC-533 (AECD-2165), June 11, 1948; and LA-707, October 28, 1948.

Our principal tool will be the theory of invariant imbedding. Rather than attempt to define precisely what turns out to be more a state of mind than anything else, we shall first give a number of applications of the methods. Subsequently, we shall try to distill the essence of these.

2. Simple Neutron Transport and Multiplication Process

Let us now describe a simple mathematical model of a neutron transport process with fission. Subsequently, we shall add a number of interesting features such as collision between neutrons, energy and time dependence, and so on. For the immediate purpose of illustrating both how the classical approach is made and how invariant imbedding techniques are used, there are great advantages to using the simplest possible version possessing certain structural properties.

As noted in the foregoing, we take the neutron to be a point particle, and we allow at the moment only one-dimensional motion along a line, or part of a line. To simplify matters still further, we assume that there is no energy dependence. As this blithe, carefree neutron moves along the line, it may suffer a collision with the constituent elements of the line. Again to simplify the algebra, we suppose that only fission collisions occur, resulting in one neutron moving to the left and one to the right. This is the only type of interaction we shall allow between the neutron and the transport medium at the moment. Furthermore, we shall suppose that there are no neutron-neutron interactions.

To make this verbiage precise, let us consider a finite interval $[0,x]$ (the reason for this apparently loose usage of x to designate an endpoint will be made clear subsequently; at the present, let us merely state that it is done with malice aforethought), a one-dimensional rod, with the following properties:

a. When a neutron traverses an infinitesimal length Δ, in either direction, there is a probability $\sigma\Delta+o(\Delta)$[30] that fission will occur.
b. When fission occurs, two neutrons are produced, one going to the right and one to the left. Each of these has the same properties as the original neutron. (See Fig. 1.)
c. There is a probability $1-\sigma\Delta+o(\Delta)$ that no interaction occurs in Δ, which means no change in the direction of the neutron.
d. When a neutron leaves the rod, it cannot return and it has no further effect upon the transport process.

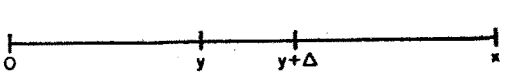

FIG. 1. A rod of length x.

[30] The notation $f(x)=o[g(x)]$ is used to mean $\lim f(x)/g(x)=0$, where the sense of the limit is usually obvious from the context.

It would not be difficult to include absorption effects and collisions, which merely change direction, or to allow R neutrons $R\neq 2$ out of a collision. Since these effects are treated subsequently in multiple scattering, radiative transfer, and random walk, we shall omit them here to keep the analytic details to an irreducible minimum.

The quantity σ is called the "macroscopic cross section." Occasionally, we shall write it as $1/\lambda$, where λ is called the "mean free path." If the rod is homogeneous, these quantities are constant, otherwise we write $\sigma(y)$ and $\lambda(y)$ for the quantities associated with the interval $[y, y+\Delta]$.

We shall begin by considering steady-state neutron flux. The more general time-dependent case will be considered below. Let a unit flux of neutrons (that is, one neutron per unit time) be incident upon the right end of the rod, and let it be desired to determine the right and left fluxes at any internal point y, as well as the fluxes out at zero and x. We shall regularly refer to the latter as transmitted and reflected fluxes, respectively.

Our first formulation will be the classical one, resulting in simple versions of the linearized Boltzmann equation.

Introduce the functions

$$\begin{aligned} u_R(y) &= \text{the expected number of neutrons going to the right at } y \text{ per unit time,} \\ u_L(y) &= \text{the expected number of neutrons going to the left at } y \text{ per unit time.} \end{aligned} \tag{1}$$

To obtain differential equations for u_R and u_L, we apply simple conservation laws for the right- and left-hand flows at y. These are input-output equations expressing the fact that what goes out is the sum of what comes in and what is produced.

By virtue of our assumptions concerning the transport and fission process and the elementary laws of probability, we obtain the equations

$$\begin{aligned} u_R(y) &= u_R(y-\Delta)(1-\sigma\Delta)+[u_R(y)+u_L(y)]\sigma\Delta+o(\Delta), \\ u_L(y) &= u_L(y+\Delta)(1-\sigma\Delta)+[u_R(y)+u_L(y)]\sigma\Delta+o(\Delta). \end{aligned} \tag{2}$$

If we pass to the limit as $\Delta\to 0$, we obtain the system of differential equations

$$\begin{aligned} u_R'(y) &= \sigma u_L(y), \\ u_L'(y) &= -\sigma u_R(y). \end{aligned} \tag{3}$$

The boundary conditions are

$$\begin{aligned} u_L(x) &= 1, \\ u_R(0) &= 0. \end{aligned} \tag{4}$$

These express the fact that there is an incident flux of unit strength at the point x, and the fact that there is no incident flux at the point 0. Observe a property which we shall repeatedly stress: The physical process

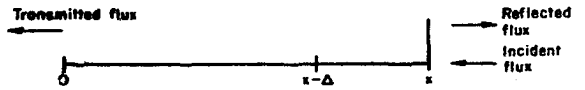

FIG. 2. The fluxes under consideration.

automatically leads to a two-point boundary value problem when formulated in the foregoing way. The reason for discussing this fact will be discussed in detail later.

Finally, let us note that we can obtain the most general second order Sturm-Liouville equation from the foregoing process if we assume that right-hand motion at y has a different mean-free path than left-hand motion and that these mean free paths vary with y.

3. Invariant Imbedding Approach—Metaphysical

We now wish to formulate the transport process described in the foregoing section in different terms. Our approach will be based upon the theory of invariant imbedding. What we wish to do is to imbed the particular process considered above within a family of processes of similar nature. Although this appears to complicate rather than simplify the problem, its justification lies in the fact that there will exist simple relations between various members of the family which can be utilized to determine the characteristics of a particular member of the family.

The fact that the structure, or anatomy, of a particular organism can be understood quite readily in terms of the comparative anatomy of a phylum is well established in the field of biology. In chemistry, the construction of the Mendelieff-Moseley periodic table of the elements was a decisive step forward. In mathematics, the method of continuity is one of the basic devices of analysis and geometry. It follows that in pursuing this approach, we are invoking a factotum of science.

Consider the way in which an experimental physicist might study neutron flux in a rod. Starting with a rod of fixed length, he would measure reflected and transmitted fluxes. Increasing or decreasing the length, measurement would be made of the corresponding quantities. The final data would consist of two curves, one the reflected flux as a function of the length of the rod, the other the transmitted flux. These would be functions of x, the length of the rod.

Our aim here is to carry out the analytic equivalent of this program. In order for these concepts to be meaningful, we must find a way of relating the reflected and transmitted flux for a rod of length x with the corresponding fluxes for rods of different length. We propose then to consider the set of processes obtained by letting x assume any positive value. Our choice of the symbol x obviously presages this development.

One advantage of this approach as far as reduction of data is concerned is that it permits a direct comparison of analytic results with experimental results. The analytic and computational advantages will be discussed *in extenso* after we have supplied some analytic content to this metaphysical discourse.

4. Invariant Imbedding Approach—Analytical

We begin by introducing the function

$u(x)$ = the expected number of neutrons reflected from $[0,x]$ per unit time as a result of an incident unit flux of neutrons per unit time at x. (See Fig. 2.)

Let us take Δ to be an infinitesimal. As the incident flux passes through the segment $[x-\Delta, x]$, some of the neutrons cause fission and others pass through unaffected to become incident upon $[0, x-\Delta]$. When a fission occurs in Δ one fission neutron emerges at x, while the other becomes a part of the incident flux at $x-\Delta$.

Some of the neutrons reflected from $[0, x-\Delta]$ may cause fission while passing through $[x-\Delta, x]$. The products of this fission yield a contribution to the reflected flux at x and furnish another source of neutrons incident upon $[0, x-\Delta]$.

Fortunately, although the physical process and mathematical counterpart are exceedingly complex if account of all fissions and reflections is taken, this intricate bookkeeping is unnecessary if Δ is an infinitesimal. All other events, apart from those taken account of above, have a probability of occurrence of order Δ^2 or higher. Hence, they can be neglected in the derivation of the differential equations for the expected flux $u(x)$. If we add up the various effects and their associated probabilities, we obtain the equation

$$u(x)=\sigma\Delta[1+u(x-\Delta)] + (1-\sigma\Delta)\big[u(x-\Delta)\{(1-\sigma\Delta) +\sigma\Delta[1+u(x-\Delta)]\}\big]+o(\Delta). \quad (2)$$

If we let $\Delta \to 0$, we derive the differential equation

$$u'(x)=\sigma[1+u^2(x)], \quad u(0)=0. \quad (3)$$

This first-order nonlinear differential equation is called a Riccati equation. As we shall see, this type of quadratically nonlinear equation is characteristic of the equations derived by invariant imbedding techniques. In contrast, the classical equations are linear. Since we are describing the same process in different ways, there must be relations between the analytic descriptions. We shall obtain these later.

A further useful function is

$v(x)$ = the expected transmitted flux per unit time as a result of a unit flux per unit time incident at x.

The same reasoning as in the foregoing shows that $v(x)$ satisfies the equation

$$v'(x)=\sigma u(x)v(x), \quad v(0)=1. \quad (5)$$

Observe that $u(x)$ satisfies a nonlinear differential equation whose solution is determined by an initial con-

dition as compared to the linear equations for $u_R(y)$ and $u_L(y)$, determined by a two-point condition.

5. Connection between the Two Approaches

It is clear that by suitable choice of y, we can obtain the functions $u(x)$ and $v(x)$ from the functions $u_R(y)$ and $u_L(y)$. Thus, if we make the dependence upon x explicit, we have

$$\begin{aligned} u_R(y) &= u_R(y;x), \\ u_L(y) &= u_L(y;x), \end{aligned} \tag{1}$$

and

$$\begin{aligned} u(x) &= u_R(x;x), \\ v(x) &= u_L(0;x). \end{aligned} \tag{2}$$

Can we, however, derive the internal fluxes $u_R(y)$ and $v_R(y)$, given the functions $u(x)$ and $v(x)$?

To accomplish this, we combine both viewpoints. Consider Fig. 3.

To obtain a relation between $u_R(y)$, $u_L(y)$, and $u(y)$, we consider a source of strength $u_L(y)$ per unit time at y. Then the steady-state relation is clearly

$$u_R(y) = u_L(y)u(y). \tag{3}$$

Similarly,

$$u_L(y) = v(x-y) + u(x-y)u_R(y). \tag{4}$$

Hence, on solving for $u_R(y)$ and $u_L(y)$, we have

$$\begin{aligned} u_R(y) &= u(y)v(x-y)/[1-u(y)u(x-y)], \\ u_L(y) &= v(x-y)/[1-u(y)u(x-y)]. \end{aligned} \tag{5}$$

It follows that we can consider $u(x)$ and $v(x)$ as fundamental functions from which all other functions can be derived.

6. Semigroup Properties[31]

Let us now obtain general relations connecting $u(x)$ and $v(x)$ with $u(y)$, $v(y)$ and $u(x-y)$, $v(x-y)$. The differential equations of Sec. 4 are particular cases of these relations.

Referring to Fig. 3 and tracing the multiply reflected and transmitted fluxes, we see that

$$\begin{aligned} u(x) &= u(x-y) + v(x-y)u(y)v(x-y) \\ &\quad + v(x-y)u(y)u(x-y)u(y)v(x-y) + \cdots \\ &= u(x-y) + \{v^2(x-y)u(y)/[1-u(y)u(x-y)]\}, \end{aligned} \tag{1}$$

and similarly

$$v(x) = v(x-y)v(y)/[1-u(y)u(x-y)]. \tag{2}$$

Two values of particular interest are $y=\Delta$ and $y=x-\Delta$. The value $y=x-\Delta$ leads, as $\Delta \to 0$, to the

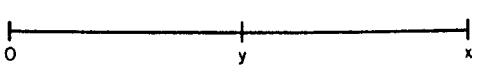

FIG. 3. Subdivision of a rod of length x.

[31] For a definition and discussion of semigroups see footnote reference 1.

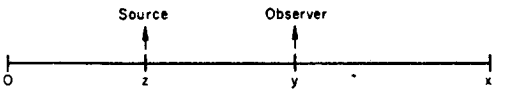

FIG. 4. Locations of source and observer.

foregoing differential equations, and the value $y=\Delta$ to Stokes' relations,[32] a matter we shall discuss again later.

These results show that we can replace the solution of differential equations by the iteration of simple transformations. Consequently, these relations may be better suited for computational purposes than the foregoing differential equations.

7. A More General Imbedding

The foregoing results have essentially been consequences of the observation that the internal fluxes $u_R(y)$ and $u_L(y)$ are functions not only of y, the position at which they are measured, but also of x, the length of the rod. Hence, we should write, as already noted in Sec. 5,

$$\begin{aligned} u_R(y) &= u_R(y;x), \\ u_L(y) &= u_L(y;x). \end{aligned} \tag{1}$$

Consider now the more general situation in which we measure the fluxes at y resulting from a source at an internal point z. (See Fig. 4.) The right-hand flux at y should now be denoted by $u_R(x,y,z)$ and the left-hand flux by $u_L(x,y,z)$. We are now at liberty to allow x, y, and z to vary, either independently one at a time, or two at a time, or all three together.

We see then that there are at least three different ways in which we can imbed a particular process within a family of processes. Two of these, variation of y and z, lead to linear equations with two-point boundary conditions, while the third, variation with respect to x, leads to a nonlinear equation with an initial value condition. Each has certain analytic and computational advantages. In any particular situation, we employ the formulation which is most convenient.[33]

8. Energy Dependence (Multigroup Theory)[34]

Let us now turn our attention to a more realistic mathematical model in which we assume that a neutron is characterized by an energy level as well as a direction. In so doing, we have our choice of either a continuous range of energies, or a finite set of discrete levels.

We have already discussed the continuous version.[33] Let us concentrate upon the discrete version here, since this is a case of greater importance from the computational point of view. We shall begin, as before, with the conventional formulation.

[32] F. Jenkins and H. White, *Fundamentals of Optics* (McGraw-Hill Book Company, Inc., New York, 1950), pp. 199–201.

[33] R. Bellman, R. Kalaba, and G. M. Wing, J. Math. and Mech. 7, 741 (1958).

[34] R. Bellman and R. Kalaba, "Transport theory and invariant imbedding," *Proc. Symposium on Reactor Theory* (American Mathematical Society, Providence, Rhode Island), to be published.

The internal flux at y is now described by two vectors

$$u(y)=\begin{bmatrix} u_1(y) \\ u_2(y) \\ \vdots \\ u_N(y) \end{bmatrix}, \quad v(y)=\begin{bmatrix} v_1(y) \\ v_2(y) \\ \vdots \\ v_N(y) \end{bmatrix}, \tag{1}$$

where N is the number of distinct energy levels or groups, $u_i(y)$ represents the flux of neutrons in the ith level to the right, and $v_i(y)$ the corresponding flux to the left.

Generalizing the foregoing model of a neutron transport process, we suppose that various interactions such as absorption, fission and nonfission collisions and so on, result in neutrons at one energy level being transformed into neutrons at other levels.

We introduce four matrices

$$A=(a_{ij}), \quad B=(b_{ij}), \quad C=(c_{ij}), \quad D=(d_{ij}), \tag{2}$$

where

$a_{ij}\Delta=$ the expected *incremental* number of neutrons at the ith level in the right-hand flux at $y+\Delta$, per neutron at the jth level in the right-hand flux at y, (3)

to within terms of order magnitude $0(\Delta)$. Similarly, $b_{ij}\Delta$ denotes the incremental contribution from left-hand to right-hand flux, $c_{ij}\Delta$ from right-hand flux to left-hand flux, and $d_{ij}\Delta$ from left-hand flux to left-hand flux. It should be noted that in the completely isotropic case the matrices A, B, C, D are closely related.

The usual conservation considerations lead to the equations

$$\begin{aligned} u_i(y+\Delta)-u_i(y)&=\Delta\sum_{j=1}^{N} a_{ij}u_j(y) \\ &\quad +\Delta\sum_{j=1}^{N} b_{ij}v_j(y)+0(\Delta), \\ v_i(y)-v_i(y+\Delta)&=\Delta\sum_{j=1}^{N} c_{ij}u_j(y) \\ &\quad +\Delta\sum_{j=1}^{N} d_{ij}v_j(y)+0(\Delta), \end{aligned} \tag{4}$$

for $i=1, 2, \cdots, N$.

Letting $h\to 0$, we obtain the following vector-matrix equations:

$$\begin{aligned} du/dy&=Au+Bv, \\ -(dv/dy)&=Cu+Dv, \end{aligned} \tag{5}$$

for $0\leq y\leq x$.

As before, let us suppose that no neutrons are incident at 0, and there is a flux of intensity b_i per unit time of neutrons in the ith level at x. We thus obtain the two-point boundary conditions

$$u(0)=0, \quad v(x)=b. \tag{6}$$

If the rod is inhomogeneous, the matrices A, B, C, and D will depend upon y. Although there is no difference as far as the functional equation technique of invariant imbedding is concerned between the treatment of the homogeneous and inhomogeneous, the classical treatment is simplified by the assumption of constancy of A, B, C, and D. The discussion below applies equally to constant or variable matrices.

Let $W(y)$ be the matrix solution of

$$\frac{dW}{dy}=\begin{bmatrix} A & B \\ -C & -D \end{bmatrix}W, \quad W(0)=I. \tag{7}$$

To solve (5) subject to (6), we suppose that $v(0)$ has the as yet unknown value c. Then, the solution of (5) can be written

$$\begin{bmatrix} u(y) \\ v(y) \end{bmatrix}=W(y)\begin{bmatrix} 0 \\ c \end{bmatrix}. \tag{8}$$

Write

$$W(y)=\begin{bmatrix} W_{11}(y) & W_{12}(y) \\ W_{21}(y) & W_{22}(y) \end{bmatrix}, \tag{9}$$

where each W_{ij} is an $N\times N$ matrix. If we use the terminal condition $v(x)=b$, we obtain the equation

$$W_{22}(x)c=b, \tag{10}$$

which determines the unknown vector c.

9. Computational Aspects

The determination of c in (8.10) requires the solution of a system of N linear equations in N unknowns. In addition, we must determine the $N\times N$ matrix W using the linear differential equation of footnote reference 7. Fortunately, since the equation is linear, we can determine $W(x)$ one column at a time. Hence, instead of the simultaneous determination of N^2 functions, we can perform N determinations of N functions.

10. Reflection and Transmission Matrices

Let us now consider the foregoing process using invariant imbedding techniques. To that end we introduce the matrix $R(x)=[r_{ij}(x)]$, where

$r_{ij}(x)=$ the expected flux of neutrons in state i reflected per unit time from a rod of length x resulting from an incident flux at x of unit intensity per unit time in state j. (1)

The same type of reasoning employed in the one-dimensional case yields the matrix equation

$$\begin{aligned} R(x+\Delta)=B\Delta+(I+A\Delta)R(x)(I+D\Delta) \\ +R(x)CR(x)\Delta+0(\Delta). \end{aligned} \tag{2}$$

In the limit this yields the Riccati matrix equation

$$R'(x)=B+AR+RD+RCR, \tag{3}$$

with the initial condition $R(0)=0$.

In a similar fashion, if we introduce the transmission matrix $T(x)=[t_{ij}(x)]$, where

$t_{ij}(x)$ = the expected flux of neutrons in state i transmitted per unit time through a rod of length x resulting from an incident flux at x of unit intensity per unit time in state j. (4)

Then, we obtain as before

$$T'(x)=T(D+CR). \tag{5}$$

11. Computational Aspects

The determination of $R(x)$, by way of (10.3), requires the simultaneous integration of N^2 nonlinear equations with the initial value $R(0)=0$. This is a far more complicated operation than that of solving N sets of N linear equations, but, in recompense, it avoids the task of solving N simultaneous linear equations.

Furthermore, let us note that once $R(x)$ has been determined, we have resolved the transport process, determination of internal and external fluxes, for a set of rods of increasing length. On the other hand, the conventional method based upon linear equations yields the solution for one length at a time.

12. Criticality

Let us turn to a discussion of one of the most important phenomena associated with neutron transport and multiplication, namely criticality. As the length of the rod increases, the intensity of internal and emergent flux increases and becomes infinite as a certain critical length is attained.

To determine the critical length for the energy-independent case, let us begin with the linear equations of Sec. 2. If we eliminate $u_L(y)$, we obtain the equation

$$u_R''(y)=\sigma u_L'(y)=-\sigma^2 u_R(y). \tag{1}$$

We take σ constant for simplicity. The general solution is

$$u_R(y)=c_1\sin\sigma y+c_2\cos\sigma y. \tag{2}$$

On using the two-point boundary conditions of (2.5), we readily obtain the equation

$$u_R(y)=\sin\sigma y/\cos\sigma x. \tag{3}$$

We see then that $u_R(y)$ and $u_L(y)$ are infinite for $0<y<x$ when $x=\pi/2\sigma$. This is the *critical length* for the simple neutron multiplication process we have set up.

On turning to the equation for the reflected flux obtained via invariant imbedding, we have

$$u'(x)=\sigma(1+u^2),\quad u(0)=0, \tag{4}$$

whence

$$u(x)=\tan\sigma x. \tag{5}$$

Once again, we see that $x=\pi/2\sigma$ is the critical length.

As pointed out by McGarvey, we can use (6.1) or (6.2) to obtain the critical length. In place of asking for the value of x which makes $u(x)$ infinite, it is sufficient to ask for the value of x which makes $u(x)=1$, and then double x.

13. Criticality—Multigroup Case

It is in the determination of critical length in the energy-dependent case that the classical formulation encounters real trouble. To find the value of x which yields infinite flux, we must solve the determinantal equation

$$\det[W_{22}(x)]=0. \tag{1}$$

Let us note, once and for all, that when we speak of the critical value, we mean the smallest value of x which yields an infinite flux. From the physical point of view, the problem of determining expected fluxes is meaningless when the length of the rod exceeds the critical value. The higher values of x which yield infinite values are connected with the higher characteristic values associated with the two-point boundary-value problem. They do not appear to have any physical significance, although this is always a dangerous statement.

On the other hand, when we go over to a more sophisticated discussion concerning probabilities of fluxes of various intensity, and probability of fission, then it becomes quite significant to consider rods of greater than critical length. There are a number of interesting mathematical problems in this area which have been considered in detail by McGarvey,[35] and Mullikin and Snow.[36] We shall discuss them briefly below.

Returning to the equation in (1), we see that if N, the number of groups, is of any size, say 10 or 20, the problem is not trifling. If $N=50$ or 100, we cannot consider a solution along the foregoing lines to be satisfactory, for a number of reasons which are familiar to numerical analysts.

The invariant imbedding technique requires the integration of N^2 simultaneous differential equations which are quadratically nonlinear. This integration is pursued until some element in the matrix $R(x)$ becomes infinite. To begin with, let us discuss the dimensional aspects. A computation of this type for $N=10$ or 20 is completely routine for modern digital computers, and one of this nature for $N=50$ is large, but feasible. For the machines that will be operational within a few years, values of N such as 100 or 200 will be routine.

Now let us turn to the integration of the differential equations until a singularity occurs. Clearly, this is not a routine operation if accuracy is desired. There are several things that we can do. First of all, we can observe that as x approaches x_0, the critical value, we have an asymptotic behavior of the form

$$r_{ij}(x)\sim s_{ij}/(x-x_0), \tag{2}$$

[35] D. McGarvey (to be published).
[36] T. Mullikin and R. Snow (unpublished).

where $s_{ij} \geq 0$, and some $s_{ij} > 0$. Hence

$$1/r_{ij}(x) \sim (x - x_0)/s_{ij}, \tag{3}$$

when $s_{ij} > 0$. This linear behavior can be used to predict the value of x_0 with great accuracy. Furthermore, the fact that there are N^2 functions $r_{ij}(x)$ will enable us to determine x_0 with even greater accuracy.

Secondly, we can use McGarvey's observation, pointed out in the section on criticality for the simple energy-independent case. In place of finding the first value of x for which $R(x)$ is singular, we can ask for the first value of x for which the matrix $R(x)$ has its largest characteristic root equal to one. If this value is x_1, the critical value will be $2x_1$.

Since the matrix $R(x)$ is a positive matrix, or at least, nonnegative, we know that there will be one root of largest absolute value which is real.[37] By slight perturbation of the transition matrices A, B, C, and D we can actually ensure that all the entries in $R(x)$ are positive, which means that the root with largest absolute value will actually be positive.

There are now available a number of simple and efficient techniques for determining this root, the Perron root, of a positive matrix. Furthermore, since clearly $R(x)$ has monotonically increasing elements, we can use various interpolation methods to locate the position of this root very accurately. A large number of questions in the theory of branching processes can be reduced to the problem of determining the largest characteristic roots of positive operators; see Bellman-Harris,[38] and Birkhoff.[39]

In any case, this method seems far superior to that of finding the roots of a determinantal equation of high degree. It would seem that invariant imbedding techniques have a distinct advantage as far as the determination of critical parameters is concerned.

14. Extrapolation over Multigroups

One way of determining the critical length with great accuracy is based upon the use of a large number of energy levels. It is reasonable to suspect that closer and closer values to the true value will be derived as we use finer and finer subdivisions of the energy range. Consequently, we can use the following extrapolation method. Solve the problem for $N = 10$, for $N = 20$, $N = 30$, and so on, until we reach the limits of the computer. If we use the successive values obtained for the critical length, we can extrapolate to $N = \infty$, and thereby obtain a more precise value.

Here is where an analysis of the precise asymptotic form as $N \to \infty$ will be very valuable. With the aid of an analytic representation of the critical length as a function of N, we can use superior extrapolation procedures.

Of course, it is seldom possible to obtain cross sections and other physical parameters, as continuous functions. Hence the limiting case $N \to \infty$ is often of greater mathematical interest than it is of physical importance.

15. Multidimensional Transport Theory—Slab Case

Leaving the physically cramped but mathematically comfortable confines of the one-dimensional, let us begin our investigation of the more significant multidimensional processes by considering a neutron transport process taking place in an infinite slab contained between the planes $y = 0$ and $y = x$ in three space. As usual, surrounding the slab is a vacuum which means that a neutron leaving the slab at either boundary never returns. (See Fig. 5.)

A classical formulation of this problem leads in the isotropic case to the equation

$$\frac{1}{c}\frac{\partial f}{\partial t} + \mu\frac{\partial f}{\partial y} + \sigma f = \frac{k\sigma}{2}\int_{-1}^{1} f(x,\mu',t)\,d\mu', \tag{1}$$

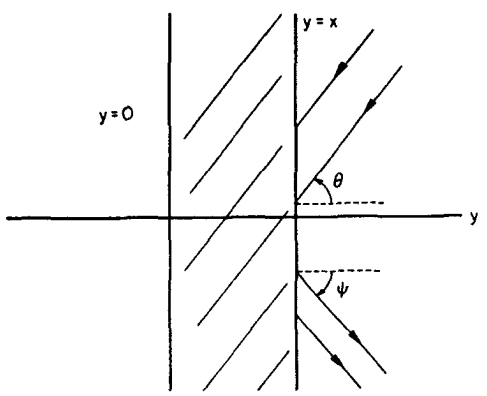

FIG. 5. The incident and reflected fluxes.

where c is the constant neutron velocity, σ is the constant collision cross section, and k is the average number of neutrons emerging from a collision. As usual, μ is the cosine of the angle between the direction of motion of the particle and the positive y direction, and $f(y,\mu,t)$ is the density of neutrons at y traveling in direction μ at time t.

There are boundary conditions at $y = 0$ and $y = x$, arising from the fact that particles may not reenter the slab once they have emerged. In the steady-state situation, of the type we have so far been considering, (1) takes the form

$$\mu\frac{\partial f}{\partial y} + \sigma f = \frac{k\sigma}{2}\int_{-1}^{1} f(x,\mu',t)\,d\mu'. \tag{2}$$

A rigorous treatment of Eqs. (1) and (2) requires deep analysis.[23,24]

Let us consider this problem using invariant imbedding techniques. To simplify our initial presentation,

[37] R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill Book Company, Inc., New York, 1960), Chap. 16.
[38] R. Bellman and J. M. Danskin, The RAND Corporation, Rep. R-256, Chap. 5, March 1, 1954.
[39] G. Birkhoff, Proc. Nat. Acad. Sci. U. S. 45, 567 (1959).

let us return to neutrons which are independent of energy, but do, however, possess directions of motion. Assume, as indicated in Fig. 5 that there is a plane-parallel flux in direction θ per unit area per unit time incident at x, and that we are given the various probabilities of absorption, scattering and fission collisions, and the resultant angular distribution of neutrons.

The type of reasoning used in the previous sections enables us to derive a functional equation of the form

$$\partial u/\partial x = T(u), \tag{3}$$

where T is a quadratic operation, for the function

$u(x,\theta,\psi)$ = the reflected flux per unit area *on the surface* in the ψ direction per unit time as a result of a unit incident flux per unit area *on the surface* per unit time.[40] (4)

There is no need for us to go into the details for three reasons. In the first place, we shall derive similar equations below for cylindrical and spherical geometries. The second reason we shall discuss immediately below. Finally, we shall discuss this problem from another physical viewpoint in Sec. V.

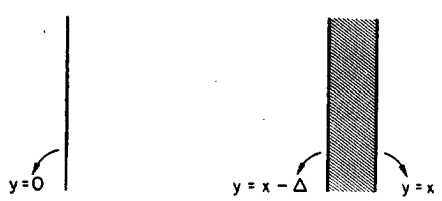

FIG. 6. A stratified slab.

16. Equivalence of One-Dimensional Energy-Dependent Cast and Angular-Dependent, Energy-Independent Slab Case

What is important is the observation that the transport process for a one-dimensional rod with energy-dependence is abstractly equivalent to the process for the slab with discrete angular dependence, but no energy dependence.

In both cases, we have a finite number of "states" and mechanisms for transforming a neutron from one state to another. Another advantage of this formulation lies in the fact that the inclusion of energy dependence in the slab merely increases the number of states, without at all changing the mathematical formulation.

17. Cylindrical Regions

The infinite slab is stratified by considering it to be composed of a series of strata of which the stratum between $y=x$ and $y=x-\Delta$ is typical (Fig. 6).

In analogous fashion, we can stratify other regions

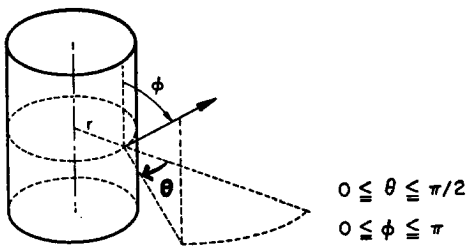

FIG. 7. A problem with cylindrical geometry.

with various types of symmetries. Consider, for our first example of this, an infinite cylindrical region, whose cross section $\sigma(r)$ is dependent only upon the radial coordinate r. Let us suppose that neutron production is energy independent and isotropic, with k neutrons emerging after each collision.

Given an incident flux of one neutron per unit area per unit time on the surface at angles (θ,ϕ), we wish to determine the reflected flux $\psi(r,\mu,\phi,\mu',\phi')$. As usual, $\mu=\cos\theta$ (Fig. 7).

The imbedding is now performed by considering the cylindrical region to be composed of a sequence of infinitesimal cylindrical shells. In cross section, they appear as in Fig. 8. (For ingoing particles, θ is measured with respect to the inward normal.) On referring to Figs. 7 and 8, and adding up effects as before, we obtain the functional equation[41]

$$\frac{d\psi}{dr}=\frac{q\sigma(r)\csc\phi}{4\pi\mu}+\frac{q\sigma(r)\csc\phi}{4\pi\mu}\int_0^{\pi}d\phi''\int_0^1\psi(r,\mu'',\phi'',\mu',\phi')d\mu''$$
$$-\frac{\sigma(r)}{4\pi}\left[\frac{\csc\phi}{\mu}+\frac{\csc\phi'}{\mu'}\right]\psi(r,\mu,\phi,\mu',\phi')$$
$$+\frac{q\sigma(r)}{4\pi}\int_0^{\pi}d\phi''\int_0^1 d\mu''\psi(r,\mu,\phi,\mu'',\phi'')\frac{\csc\phi''}{\mu'}$$
$$\cdot\left\{1+\int_0^{\pi}d\phi'''\int_0^1 d\mu'''\psi(r,\mu''',\phi''',\mu',\phi')\right\},$$
$$\psi(0,\mu,\phi,\mu',\phi')=0. \tag{1}$$

To compute $d\psi/dr$, we must note that μ itself is really a function of r, and the same is true of μ'. Upon taking

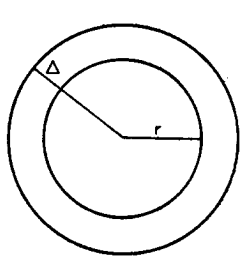

FIG. 8. Stratification of a cylinder.

[40] Throughout this paper we measure fluxes with respect to the geometrical areas on which they impinge, rather than with respect to a plane normal to the beam. For a discussion, see Sec. 59.

[41] R. Bellman, R. Kalaba, and G. M. Wing, J. Math. and Mech. 8, 575 (1959).

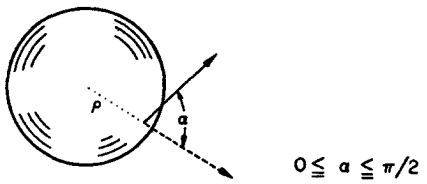

FIG. 9. A process taking place in a sphere.

this into consideration, we find

$$\frac{d\psi}{dr}=\frac{\partial\psi}{\partial r}+\frac{\partial\psi}{\partial\mu}\frac{1-\mu^2}{\mu r}+\frac{\partial\psi}{\partial\mu'}\frac{1-\mu'^2}{\mu' r}. \tag{2}$$

We shall discuss the corresponding result for spherical regions, and then discuss the computational significance of these results.

18. Spherical Regions

As our next example, consider a sphere composed of transport material whose cross section is dependent upon the radial coordinate ρ alone. As indicated in the following figure, we introduce an angular coordinate α, $\cos\alpha=v$, and suppose that we have a conical flux of neutrons, with direction v, incident uniformly over the surface of the sphere, one neutron per unit area per unit time. We wish to determine the reflected flux in direction v', $\psi(\rho,v,v')$. (See Fig. 9.)

The usual analysis yields the equation[41]

$$\frac{\partial\psi}{\partial\rho}+\frac{1-v^2}{v\rho}\frac{\partial\psi}{\partial v}+\frac{1-v'^2}{v'\rho}\frac{\partial\psi}{\partial v'}$$

$$=\frac{q\sigma(\rho)}{4\pi v}+\frac{q\sigma(\rho)}{2v}\int_0^1\psi(\rho,v'',v')dv''$$

$$-\sigma(\rho)\left(\frac{1}{v}+\frac{1}{v'}\right)\psi(\rho,v,v')+\frac{q}{2}\sigma(\rho)\int_0^1 dv''\frac{\psi(\rho,v,v'')}{v''}$$

$$\times\left\{1+2\pi\int_0^1\psi(\rho,v''',v')dv'''\right\}. \tag{1}$$

19. Critical Mass

The critical reader may seriously question the value of the results obtained in the two previous sections, since incident fluxes of the type we have employed are seldom found. This is certainly a valid criticism.

There is, however, one quite important case in which we can profitably use this type of flux, and, indeed, whatever type of flux is most convenient. This is the determination of critical mass. It is possible to convince oneself that whatever radius is critical for one type of flux will be critical for any other type of steady-state flux.

20. More General Fluxes

The same persevering reader may also ask why we have not used invariance principles directly for more general fluxes. This can be done. What has held us back has been dimensionality difficulties. Consider, for example, a two-dimensional slab in which we consider an incident flux of unit intensity per unit time at an angle θ at a particular point, say $z=0$. (See Fig. 10.) We then introduce the flux, $u(\theta,\psi,z,x)$, as the reflected flux at angle ψ per unit time at the point a distance z from the point of incidence. We then obtain the same type of equation for u as before, with the difference that u now depends upon one additional variable z. This increase in dimensionality introduces formidable computational difficulties due to the enormously increased memory requirements.

From the analytic point of view, there is no difficulty in considering realistic fluxes. From the computational point of view, these more realistic problems require new techniques and bigger and faster machines. For a possible line of approach, see Bellman and Dreyfus.[42]

21. Volterra vs Fredholm Equations

The equations we have obtained in the foregoing sections using invariant imbedding techniques have invariably been nonlinear, as compared to the linear equations of classical transport theory. Considering the fact that linear equations with their superlative superposition properties are difficult enough to analyze theoretically and resolve numerically, why do we wish to introduce nonlinear equations? Although we have gnawed around the edges of this question in previous pages, let us now make it the principal course.

Our answer can be put in very simple terms: We wish uniformly to replace two-point boundary-value problems, and boundary-value problems in general, by initial value problems. This is equivalent to replacing Fredholm-type integral equations by Volterra-type integral equations. Naturally, the equations will be in different variables.

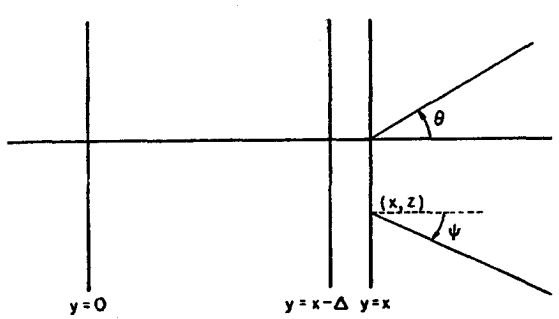

FIG. 10. Incident and reflected fluxes.

[42] R. Bellman and S. Dreyfus, "Functional approximations and dynamic programming," *Math. Tables and other Aids to Comp.* (1959).

This is not a new idea, and, indeed, is one that has been proposed before, and used with some success. The approach we use, however, based upon invariance principles, and extending that of Ambarzumian[6] and Chandrasekhar,[5] is quite different from these mentioned, and quite unlike any earlier methods.

We are engaged in this program for two reasons. In the first place, Volterra-type equations lead to iterative algorithms which are simpler for digital computers than algorithms based upon the solution of linear systems of equations. Secondly, and the two are intimately related, functional equations of the type we derive, despite their nonlinearity, are easier to treat as far as existence and uniqueness are concerned. These last topics, however, we have bypassed here since we are at the moment principally interested in exhibiting the mechanics of the formulation of the classical particle processes in these new terms.

22. Stokes Relations

It is interesting to find that the reflection and transmission matrices, and, more generally, the reflection and transmission functions, are related to each other in algebraic fashion. We already have the Riccati differential equation for $R(x)$ and the differential equation for $T(x)$ in which $R(x)$ enters (see Sec. 10).

We shall refer to these new relations as Stokes' relations since the first identities of this type connecting reflection and transmission coefficients were discovered by Stokes in work on light rays impinging on slabs.

In Sec. 6, we discussed the semigroup properties of the functions $u(x)$ and $v(x)$ obtained for the simple one-dimensional energy-independent process. Recognition of these transformation properties is also found in Redheffer.[43] and for the matrix case as well. To obtain the following relations, we use the special case of these relations in which the stratification instead of being as before like Fig. 11, is, instead, like Fig. 12, where Δ is an infinitesimal.

The usual counting process yields the relation

$$R(x+\Delta)=R(x)+T(x)BT(x)\Delta+0(\Delta), \tag{1}$$

or

$$R'(x)=TBT. \tag{2}$$

For simplicity we assume that

$$A=D, \quad B=C. \tag{3}$$

In view of Eq. (10.3), we conclude that

$$TBT=B+DR+RD+RCR, \tag{4}$$

a relation which is not too easy to verify directly.

FIG. 11. One stratification of a rod.

[43] R. Redheffer, in *Mathematics for Modern Engineers* (1960), Vol. 2.

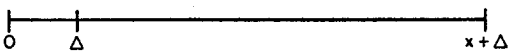

FIG. 12. A second stratification of a rod.

Similarly, we find that

$$T(x+\Delta)=(I+D\Delta)T(x)+R(x)BT(x)\Delta+0(\Delta), \tag{5}$$

whence

$$T'(x)=(D+RB)T. \tag{6}$$

This in conjunction with Eq. (10.5) yields the further result

$$T(D+BR)=(D+RB)T. \tag{7}$$

23. Probabilities

For various purposes, it is desirable to have a more precise picture of the transmitted and reflected flux than that furnished by the expected values. This is particularly the case when x is just less than critical, when it assumes the critical value, and when x is greater than critical, the case of *supercriticality*.

Let us then talk about the probabilities of events, rather than the expected events. In place of a steady-state situation, let us suppose that one neutron is incident at x, the right end of our one-dimensional rod, at time zero. We shall call this neutron the *trigger neutron*.

Let us define the set of probabilities

$$p_n(x)=\text{the probability that } n \text{ neutrons are reflected from a rod of length } x \text{ over all time as a result of one trigger neutron incident at } x \text{ at time zero.} \tag{1}$$

In order to obtain a set of differential equations for these functions, we observe that the trigger neutron incident upon a rod of length $x+\Delta$ either has a fission collision in the initial length $[x+\Delta, x]$ or it does not. If it does not, consider the neutrons that emerge from the length $[0,x]$. If k of these emerge over all time, then at most one of these, to terms in $0(\Delta)$, can have a fission collision in the interval $[x, x+\Delta]$. Consideration of these possibilities, together with that of an initial fission collision, leads to the relation

$$p_n(x+\Delta)=(1-\sigma\Delta)\times\{p_n(x)(1-n\sigma\Delta)+\sum_{k=1}^{n} p_k(x)k\sigma\Delta p_{n-k}(x)\}+\sigma\Delta p_{n-1}(x)+0(\Delta),$$
$$n=0, 1, 2, \cdots; \quad p_{-1}(x)=0. \tag{2}$$

Passage to the limit yields the infinite system of differential equations

$$p_n'(x)=-(n+1)\sigma p_n(x)+\sigma p_{n-1}+\sigma\sum_{k=1}^{n} kp_k(x)p_{n-k}(x),$$
$$n=0, 1, 2, \cdots; \quad p_{-1}(x)=0. \tag{3}$$

Physical considerations yield the obvious boundary conditions

$$p_n(0)=\begin{cases}1, & n=0\\ 0, & n\neq 0.\end{cases} \tag{4}$$

In order to test the feasibility of the computational solution of systems of this type, and to obtain some idea of the time required, the first forty of these equations were solved numerically using a rather old-fashioned machine, the Rand Johnniac.[34,44]

A number of interesting questions concerning the analytic behavior of the $p_n(x)$ as x approaches the critical value arise as a result of these computations.

If we introduce the generating function

$$u(x,s)=\sum_{n=0}^{\infty} p_n(x)s^n, \tag{5}$$

we readily obtain the quasilinear partial differential equation

$$u_x=\sigma(s-1)u+\sigma s(u-1)u_s, \tag{6}$$

with the initial condition

$$u(0,s)=1. \tag{7}$$

This equation has been studied in detail by Mullikin and Snow.[36] The solution exhibits a very strange behavior as x goes through the critical value. As we shall see later, the equation for the generating function can be obtained immediately by means of functional equation techniques.

It is important to insert a word of caution about the use of these techniques. Methods based upon expected values can be used with a carefree abandon as long as the length of the rod is less than critical. On the other hand, the probabilistic equations obtained in the foregoing hold for any value of the rod. They must be considered the basic equations.

As long as x is less than the critical length, we have the condition

$$\sum_{n=0}^{\infty} p_n(x)=1, \tag{8}$$

in addition to the initial values of (4). As soon as x is greater than the critical length, this equation no longer holds. This is caused by the fact that there is now a new probability to be added, the probability of an infinite flux. Lack of recognition of this fact can lead to paradoxical conclusions. A thorough discussion of this phenomenon will be found in the paper by Mullikin and Snow cited in the foregoing.

Finally, let us note that similar equations can be obtained for the transmission probabilities.[44]

24. Analogy between Critical Length and Initiation of Shock Wave

The equation for the generating function, given in Sec. 23, is analogous to the equation

$$u_t=uu_x, \tag{1}$$

where t is now a time variable and x a space variable, used by Courant-Hilbert, and others, as an example of how a discontinuity can arise in the behavior of the solution of a differential equation. This type of discontinuity is similar to that which is observed in the behavior of blast waves and is called a "shock."

It is interesting then to observe this analogy between the onset of a shock as a function of *time* and the onset of criticality as the length, or radius, is increased. Analogies of this type are useful since knowledge gained in one area can then be easily transplanted to another.

We shall observe a further analogy subsequently. Just as the presence of the smallest degree of viscosity destroys the pure shock, so the presence of the slightest neutron-neutron interaction can destroy criticality.[45]

25. Description of a Generalized Transport Process

As we shall see in a moment, the imbedding technique, which we have used so far only for one-dimensional rods, slabs, cylindrical and spherical regions, can be considerably extended. Let us now formulate a transport process in general terms. Let a family of surfaces in n-dimensional space be characterized by a single continuous parameter $\eta\geqq 0$. The surface corresponding to $\eta=0$ (it may be a degenerate surface) will be considered a bounding surface, and the parametrization will be such that the region included between $\eta=0$ and $\eta=\eta_1$ will be included by the region between $\eta=0$ and $\eta=\eta_2>\eta_1$. It is clearly not necessary to consider the topological properties of these surfaces and regions in detail. Such ideas as outward and inward directions, area of a surface, and so on, can be taken intuitively as far as our purposes are concerned. The family of surfaces will be assumed to partition continuously all or part of the n-dimensional space into a set of strata.

For example, the family of surfaces may be the set of all spheres centered at the origin in three-dimensional space. Here η is r, the radius of the sphere, and $\eta=0$ is a degenerate bounding surface, a point sphere. Again, the family may be the set of all vertical lines, in the two-dimensional space, to the right of the vertical axis. In this case we can choose η to be x, and $x=0$ is a non-degenerate bounding surface.

By a "particle" we shall understand a state vector S depending on the parameter η. The state vector contains information regarding the direction of motion, energy, specific location on η, the type or types of physical

[44] R. Bellman, R. Kalaba, and G. M. Wing, J. Math. and Mech. 7, 149 (1958).

[45] R. Bellman, R. Kalaba, and G. M. Wing, J. Math. and Mech. 8, 249 (1959).

particles that we are discussing (in case there are particles other than neutrons), and any other properties which we may choose to include in the process.

The stratum $(\eta, \eta+\Delta)$, $\Delta>0$, will be assumed to contain a medium which permits a transport process. A particle passing through the stratum may engage in interactions of both a deterministic and a stochastic nature. As mentioned above, the distinction between these is really a matter of mathematical convenience. The deterministic interactions will produce effects which will be proportional in magnitude to Δ plus a term $0(\Delta)$; the stochastic interactions will have *probability* of occurrence proportional to Δ plus $0(\Delta)$ within the stratum $(\eta, \eta+\Delta)$. These interactions will have no effect on the transport medium, but will result in a transformation on the state vector S, in some cases transforming it into two or more such vectors (fission), in some cases annihilating it (absorption), in other cases leaving one vector as before. Hence, the movement of a particle within the medium between 0 and η can be thought of as a sequence of transformations on state vectors, together with the creation and annihilation of vectors. Subsequently, in Sec. 36, we shall consider a process in which the medium is changing as the process continues.

We shall now investigate the following problem. Let a flux of "particles" specified by S impinge on η. What are the number and nature of the particles (state vectors) emergent from η? Often the source will be given in particles per unit time, in which case we shall seek the number of particles emerging from η per unit time. In some instances, we shall be concerned with the number and nature of particles emergent from $\eta=0$ per unit time? The former particles we shall call "reflected," the latter we call "transmitted." It is clear that in some cases, such as for the sphere mentioned above, the second problem is ill-posed. We shall investigate only the problem of reflection, since the formulas for transmission can be obtained in a similar fashion.

26. Expected Value Equation

We begin by considering not the state vector itself, but its expected value. Consider a stream of particles, one per unit area per unit time, in state S, impinging upon the surface η. We ask for the expected number, or flux, of particles in state S' reflected per unit area per unit time. Denote this flux by $\psi(\eta,S,S')$. For the present discussion we shall assume that S and S' contain no information about the specific location on η. It is evident that this assumption imposes a strong symmetry requirement upon both the surface η and the impinging flux.

Let the probability that a particle in state S passing through $(\eta, \eta\pm\Delta)$ suffers a collision—the stochastic process—be given by $P(\eta,S)\Delta+0(\Delta)$. Let $T(\eta,S,S')$ be the average number of particles in state S' resulting from this interaction and transmitted to $\eta\pm\Delta$. Let $R(\eta,S,S')$ be the average number in state S' reflected back to η. Then, proceeding as in the foregoing, we find

$$\begin{aligned}
&\psi(\eta+\Delta, S, S') \\
&\quad = P(\eta,S)\Delta R(\eta,S,S') \\
&\qquad + P(\eta,S)\Delta \int_{S''} T(\eta,S,S'')\psi(\eta,S'',S')dS'' \\
&\qquad + [1-P(\eta,S)\Delta]\psi(\eta,S,S')[1-P(\eta,S')\Delta] \\
&\qquad + [1-P(\eta,S)\Delta]\int_{S''} dS''\psi(\eta,S,S'')\Delta P(\eta,S'') \\
&\qquad \cdot \left\{ T(\eta,S'',S') + \int_{S''} R(\eta,S'',S''') \right. \\
&\qquad\qquad \left. \times\psi(\eta,S''',S')dS''' \right\} + 0(\Delta). \quad (1)
\end{aligned}$$

The first term on the right-hand side of this equation represents the contribution to the reflected flux from the particles which are reflected immediately from the stratum of thickness Δ, and the second arises from those which pass through this stratum but change state, giving reflected particles from $[0,\eta]$ which then pass through the stratum without interaction. The third term is produced by particles which pass unaffected through $[\eta, \eta+\Delta]$ and give rise to reflected particles from $[0,\eta]$ which again pass through the stratum without interaction. The last term accounts for particles which enter $[0,\eta]$ without interaction in $[\eta, \eta+\Delta]$, but whose reflected flux does have an interaction in $[\eta, \eta+\Delta]$. Some of this flux is transmitted through this stratum, the rest is returned to $[0,\eta]$ and re-reflected.

Here all the states on the right-hand side are taken at η, and the integration over states is symbolic. The transport equation resulting when $\Delta \to 0$ is then

$$\begin{aligned}
&\frac{\partial\psi}{\partial\eta} = P(\eta,S)R(\eta,S,S') + P(\eta,S) \\
&\qquad \times \int_{S''} dS''T(\eta,S,S'')\psi(\eta,S'',S') \\
&\qquad - [P(\eta,S)+P(\eta,S')]\psi(\eta,S,S') \\
&\qquad + \int_{S''} dS''\psi(\eta,S,S'')P(\eta,S'') \left\{ T(\eta,S'',S') \right. \\
&\qquad\qquad \left. + \int_{S'''} dS'''R(\eta,S'',S''')\psi(\eta,S''',S') \right\}. \quad (2)
\end{aligned}$$

It may be shown that (2) includes Eqs. (17.1) and (18.1) as special cases. By choosing different geometries and different meanings for S, it is possible to write down a great variety of particular transport equations using this general result. For more details, see footnote 4.

27. Simple Stochastic Case

Before attempting to write down a general stochastic functional equation, we consider a simple example, the first of Sec. 2. We assume, for further simplicity, that in a collision *exactly* two neutrons emerge, one going to the right, one to the left. We let one neutron enter the bar at time zero.

Let $\{U^{(i)}(x)\}$, $i=1, 2, 3, \cdots$, be a sequence of random variables denoting the number of neutrons reflected from the bar in all time. Let $\{F^{(i)}(\Delta)\}$, $i=1, 2, 3, \cdots$, be another sequence of random variables with

$$F^{(i)}(\Delta)=\begin{cases}1 & \text{if a collision occurs in a segment of length } \Delta,\\ 0 & \text{otherwise.}\end{cases}$$

(See Fig. 15.) Then, using the invariant imbedding principle, we have

$$U^{(1)}(x)=F^{(1)}(\Delta)\{1+U^{(2)}(x-\Delta)\}+[1-F^{(1)}(\Delta)] \times \sum_{i=4}^{U^{(3)}(x-\Delta)+4}\{1+F^{(i)}(\Delta)U^{(i)}(x-\Delta)\} +w(x,\Delta), \quad (1)$$

where $\text{Prob}\{w(x,\Delta)\neq 0\}=0(\Delta)$.

Let us interpret this equation. The superscripts in themselves have no significance and serve merely to distinguish one random variable from another. Notice that if the initiating particle makes a collision in passing from x to $x-\Delta$ (Fig. 13), the second term of (1) is zero while the first gives just the number of particles emergent from $x-\Delta$—namely, the one immediately out due to the collision in $(x-\Delta, x)$ plus the random number $U^{(2)}$ resulting from the left moving neutron acting as a source particle for the rod $(0, x-\Delta)$. If there is no initial interaction in the interval $(x-\Delta, x)$, then the first term of (1) is zero, and the second term counts. Of the random number $U^{(3)}(x-\Delta)$ of neutrons emerging from $x-\Delta$ some make no collisions in $(x-\Delta, x)$ and hence contribute only one to the sum. Others make a collision in $(x-\Delta, x)$ giving not only an immediate right traveling particle, but also a random number $U^{(i)}(x-\Delta)$ reflected from $(0, x-\Delta)$. The fact that all other processes are "unlikely" is included in the term w.

We now introduce the generating function

$$u(x,s)=E\{s^{U(x)}\}. \quad (2)$$

Then, using the properties of the generating function and writing $\text{Prob}\{F^{(1)}(\Delta)=1\}=\sigma\Delta+0(\Delta)$, we find, after careful calculation with (1), the equation

$$\begin{aligned}u(x,s)&=\sigma\Delta s u(x-\Delta, s)+(1-\sigma\Delta)\\ &\quad\times u(x-\Delta, (1-\sigma\Delta)s+\sigma\Delta s u(x-\Delta, s))+0(\Delta)\\ &=\sigma\Delta s u(x,s)+(1-\sigma\Delta)[u(x-\Delta, s)\\ &\quad+u_s(x-\Delta, s)(-\sigma\Delta s+\sigma\Delta s u)]+0(\Delta). \quad (3)\end{aligned}$$

This leads at once to the partial differential equation

$$u_x=-\sigma u+\sigma s u+\sigma s u_s+\sigma s u u_s. \quad (4)$$

This is precisely Eq. (23.5) derived there by using quite different methods, and from it may be obtained the usual flux equations for the rod case. It was first pointed out to us by T. E. Harris that the functional equation approach could be applied directly to derivation of the generating function. This is an application of a quite general principle that methods suitable for the derivation of first moments can be used almost unchanged to derive generating functions. From these, relations for the higher moments can be readily obtained. See Sec. 51 for another illustration.

28. Basic Stochastic Functional Equation

We shall now derive a basic stochastic functional equation applicable to the generalized situations described in Sec. 26. We introduce the appropriate random variables.

Let

$U(S,S',\eta)=$ random number of particles in state S' reflected from η over all time due to an initial particle in state S impinging on η at time zero. (S and S' may now include information as to the specific location on η.) (1)

$$r(S,\eta)=\begin{cases}1 & \text{if the particle in state } S \text{ is involved in an interaction in the stratum } (\eta-\Delta, \eta),\\ 0 & \text{otherwise.}\end{cases} \quad (2)$$

$$Z(S; S_1', S_2', \cdots, S_k'; \eta)=\begin{cases}1 & \text{if the result of an interaction of a particle in state } S \text{ with the medium is to produce } k \text{ particles in state } S_1', S_2', \cdots, S_k',\\ & k=1, 2, 3, \cdots,\\ 0 & \text{otherwise.}\end{cases} \quad (3)$$

By the stochastic variables $U^{(i)}$, $r^{(i)}$, $Z^{(i)}$ we shall mean respectively any of a denumerable set of variables with the properties described in the foregoing. Different superscripts will serve merely to distinguish different random variables, and sometimes they will be omitted.

Also, let $Q(S,\eta)$ denote the deterministic change in state caused by passage through the stratum $(\eta-\Delta, \eta)$. By a deterministic change we mean one that occurs by virtue of mere positive change without any interaction necessarily taking place. For example, any dependence of μ on r mentioned in Sec. 17 results in such a change.

Finally, we assume that only a finite set of states S is

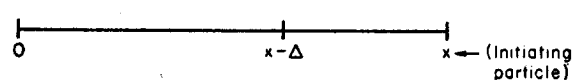

FIG. 13. A rod process.

possible. This permits us to use characteristic functions rather than characteristic functionals, and considerably simplifies the discussion.

At the risk of being somewhat redundant, we now discuss the random physical processes which occur. A particle in state S incident on the surface η enters the stratum $(\eta-\Delta, \eta)$. There it may undergo a deterministic transformation converting it from state S to state $Q(S,\eta)$. In addition, it may undergo a stochastic change (collision) producing a random number of particles in a random set of states. Each of these particles acts independently of the others and may emerge from η or be incident upon $\eta-\Delta$. In the latter case the particle is a "source" particle on $\eta-\Delta$, resulting in a random number of particles in a random set of states eventually emerging from $\eta-\Delta$. Each of these reflected particles may undergo deterministic and stochastic transformations in $(\eta-\Delta,\eta)$. Some emerge from η and are counted, others return as source particles into $\eta-\Delta$ and must be followed out again. No processes need be traced to order higher than Δ—that is, to more than one collision in $(\eta-\Delta,\eta)$.

If we enumerate these events mathematically, we arrive at the functional equation

$$\begin{aligned}U(S,S',\eta)=r(S,\eta)&\sum_{\{S_i'\}} Z(S;S_1',S_2',\cdots,S_k';\eta)\\ &\times[\sum_{i=1}^{k} U^{(i)}(S_i',S',\eta-\Delta)]\\ &+[1-r(S,\eta)]\sum_{i=1}^{n}[1-r^{(i)}(S',\eta)]\\ &+[1-r(S,\eta)]\sum_{S_m'}(\sum_{i=1}^{n'}[r^{(i)}(S_m',\eta)\\ &\times\{\sum_{\{S_i''\}} Z^{(i)}(S_m';S_i'',\cdots,S_k'';\eta)\\ &\cdot\sum_{p=1}^{k} U^{(p)}(S_p'',\bar{S}',\eta-\Delta)\}])+w(S,S',\eta),\end{aligned}\tag{4}$$

where

$$\begin{aligned}n&=U[Q(S,\eta),S',\eta-\Delta],\\ n'&=U[Q(S,\eta),S_m',\eta-\Delta],\\ \bar{S}'&\text{ is such that } S'=Q(\bar{S}',\eta),\end{aligned}$$

and $w(S,S',\eta)$ is the contribution from events that have probability $0(\Delta)$. The symbol $\{S_i\}$ means all the subsets of the set of states.

Proceeding as in Sec. 27, it is now theoretically possible to derive the flux equation of Sec. 27 by taking expected values of (4). It is likely that the direct approach of Sec. 26 is really simpler. However, the basic stochastic equation (4) seems of considerable theoretical interest and could well be used for computational purposes in place of a direct Monte Carlo approach.

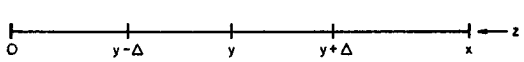

FIG. 14. The physical situation.

29. Collision Processes

So far we have not considered transport processes in which the particles interacted with each other, nor processes in which the medium was affected by the transport process. In the sections that follow, we shall consider processes of this nature.

Let us discuss a transport process in a one-dimensional rod in which we allow neutron-neutron interactions, the result being annihilation. To simplify matters, let us suppose that there is no energy dependence, and that collisions occur only between neutrons travelling in opposite directions along the line. As usual, we shall suppose that when fission occurs one neutron is produced in the forward direction and one in the backward direction.

Let

1. a. $\sigma\Delta+0(\Delta)$ = the probability that a neutron will interact with a segment of length Δ and produce fission.
   b. $u(y;x,z)$ = the expected number of neutrons per unit time passing an interior point y to the right, as a result of z neutrons per unit time introduced at x (see Fig. 14).
   c. $v(y;x,z)$ = the expected number of neutrons per unit time passing an interior point y to the left.
   d. $k(u,v)\Delta+0(\Delta)$ = the expected number of neutrons in a stream of strength u which are annihilated per unit time due to collisions with an opposing stream of strength v, in an interval of length Δ.

30. Internal Flux Equations

The usual "input-output" analysis yields the relations

$$\begin{aligned}u(y)&=u(y-\Delta)(1-\sigma\Delta)\\ &\quad+u(y-\Delta)\sigma\Delta+v(y)\sigma\Delta-\Delta k(u,v)+0(\Delta),\\ v(y)&=v(y+\Delta)(1-\sigma\Delta)\\ &\quad+v(y)\sigma\Delta+u(y)\sigma\Delta-\Delta k(u,v)+0(\Delta),\end{aligned}\tag{1}$$

where we, at this time, suppress the dependence upon x and z, and write

$$u(y,x,z)=u(y),\quad v(y,x,z)=v(y).\tag{2}$$

If we pass to the limit as $\Delta\to 0$, we are led to the nonlinear system of differential equations

$$\begin{aligned}u'(y)&=\sigma v-k(u,v),\\ v'(y)&=-\sigma u+k(u,v).\end{aligned}\tag{3}$$

The boundary conditions are

$$u(0)=0,\quad v(x)=z,\tag{4}$$

two-point boundary conditions.

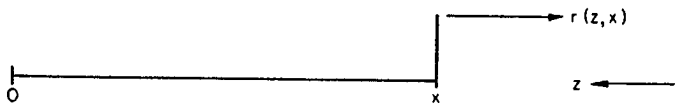

FIG. 15. The reflected flux.

31. Discussion

In general, the equations in (30.3) cannot be resolved in terms of elementary transcendents of analysis. Consequently, if we wish to obtain a numerical solution of (30.3) cum (30.4), we must resort to various computational schemes. Although a number of these are available, it cannot be said there are any of automatic application. Questions of this nature are of great difficulty, and perhaps are most easily handled by being bypassed. In the next section we shall approach this problem in a different way.

If we make the assumption that $k(u,v)=buv$, $b>0$, a certain amount of analysis can be carried out. See footnote reference 45 for some theoretical and computational results. Henceforth, we assume this form of $k(u,v)$.

32. Reflected and Transmitted Flux

Let us now approach this problem by means of functional equation techniques. Let

$$r(z,x) = \text{the expected number of neutrons reflected per unit time from a homogeneous bar of length } x \text{ as a result of having } z \text{ neutrons incident at } x \text{ per unit time.} \tag{1}$$

(See Fig. 15.)

To evaluate the expected number of neutrons reflected from a bar of length $x+\Delta$ we note, first of all, that some collisions with nucleii may occur immediately when the z neutrons enter the segment $[x, x+\Delta]$. Since each such collision results in a neutron going to the right, $\sigma z\Delta$ particles emerge at $x+\Delta$. Meanwhile, since a neutron is produced going to the left also, the original flux z is not affected by collisions with nucleii. However, this flux is *reduced* by annihilation by an amount $bzr(z;x)\Delta$ due to the opposing flux out of x. It is also *increased* by an amount $\sigma r(z;x)\Delta$ due to fission collisions in $[x, x+\Delta]$ made by the flux out of x. Hence there is at x a source of strength $z-bzr(z;x)\Delta+\sigma r(z;x)\Delta$. Finally, the reflected flux resulting from this source is partially annihilated by interactions with the impinging flux in $[x, x+\Delta]$. Summing up, we are led to the relation

$$r(z;x+\Delta) = \sigma z\Delta + r[z-brz\Delta+\sigma\Delta r(z,x)][1-bz\Delta]+0(\Delta). \tag{2}$$

By letting Δ tend to zero, we find that $r(z;x)$ satisfies the quasilinear first-order partial differential equation

$$r_x=\sigma z-bzrr_z+\sigma r r_z-bzr, \tag{3}$$

where, as usual, the subscripts indicate partial differentiation. The reflection function $r(z;x)$ also satisfies the initial condition

$$r(z;0)=0 \quad \text{and} \quad r(0;x)=0. \tag{4}$$

Equation (3) specializes, for $b=0$, to the Riccati equation derived in earlier sections for the reflection coefficient (Sec. 4). It may be resolved via characteristic theory[46] or by direct numerical integration, returning essentially to (2). The equations for the characteristics are

$$\begin{aligned} dx/ds &= 1, \\ dz/ds &= bzr-\sigma r, \\ dr/ds &= \sigma z-bzr. \end{aligned} \tag{5}$$

Since $x=s$, $z=0$, $r=0$ is a solution of the system (5) passing through the point $x=z=r=0$, we find that

$$r(0;x)=0, \tag{6}$$

as was assumed in the foregoing on physical grounds.

Once the function $r(z;x)$ has been determined for suitable ranges of z and x, one may reduce the determination of $u(y)$ and $v(y)$, the internal fluxes, to the solution of initial value problems, as was mentioned earlier. If the incident flux $v(x)=z$ is specified, then the reflected flux is $r(z;x)=u(x)$, so that now both $u(y)$ and $v(y)$ are specified at $y=x$. Through use of Eqs. (30.3) the functions $u(y)$ and $v(y)$ may now be determined on the entire interval $[0,x]$.

The equations satisfied by the transmitted flux $t(z;x)$, where

$$t(z;x) = \text{the expected number of neutrons emergent from the end } y=0 \text{ of a homogeneous bar of length } x \text{ as a result of having } z \text{ neutrons per unit time incident on the end } y=x, \tag{7}$$

are similarly derived. We have

$$t_x=(\sigma-bz)rt_z, \tag{8}$$

along with the boundary conditions

$$t(0;x)=0, \quad t(z;0)=z. \tag{9}$$

33. Discussion

Numerical solution of the foregoing Eq. (32.3), can be obtained either by use of (32.2), by means of conventional techniques, or by means of the characteristics.

In footnote reference 45 will be found a brief discussion of collision processes of this nature with energy dependence. In the remainder of this paper we consider only processes without particle-particle interaction.

[46] R. Courant and D. Hilbert, *Methoden der Mathematischen Physik* (Interscience Publishers, Inc., New York, 1937).

34. Time-Dependent Rod Case—Internal Flux

Thus far we have concentrated our attention on the stationary state in dealing with both internal and reflected and transmitted fluxes. In this section we shall obtain the equations for the internal flux in the rod, taking time variation into account. We assume that the rod has all the usual properties, and that neutrons in it travel with speed c. Thus, a time Δ/c is spent in traversing a distance Δ. It is now relatively easy to see that if

$$\begin{aligned} u(y,t) &= \text{average number of neutrons passing } y/\text{sec} \\ &\quad \text{at time } t \text{ and going to the right;} \\ v(y,t) &= \text{average number of neutrons passing } y/\text{sec} \\ &\quad \text{at time } t \text{ and going to the left;} \end{aligned} \tag{1}$$

then

$$\begin{aligned} u[y+\Delta, t+(\Delta/c)] &= u(y,t)(1-\sigma\Delta)+\sigma\Delta u(y,t) \\ &\quad +v(y+\Delta, t)\sigma\Delta+0(\Delta), \\ v[y, t+(\Delta/c)] &= v(y+\Delta, t)(1-\sigma\Delta)+\sigma\Delta v(y,t) \\ &\quad +u(y,t)\sigma\Delta+0(\Delta), \end{aligned} \tag{2}$$

giving in the limit as $\Delta \to 0$ the equations

$$\begin{aligned} (1/c)(\partial u/\partial t)+(\partial u/\partial y) &= \sigma v, \\ (1/c)(\partial v/\partial t)-(\partial v/\partial y) &= \sigma u. \end{aligned} \tag{3}$$

Equations (3) are subject to the boundary and initial conditions

$$\begin{aligned} u(0,t) &= 0, \\ v(x,t) &= 1, \\ u(y,0) &= v(y,0) = 0, \end{aligned} \tag{4}$$

for the case of the rod with a unit flux at the right end, $y=x$, imposed at $t=0$.

This formulation is the classical one. Equation (15.1) already mentioned without discussion is the analog of (3) for the more complicated geometry. Such equations as (15.1) are readily derived using the principles of this section.

35. Time-Dependent Rod Case—Reflected Flux

We now turn to a formulation of the time dependent rod problem using the basic ideas of invariant imbedding. Let us consider a single "trigger" neutron entering the rod at x at time $t=0$. It is then convenient to introduce

$$\begin{aligned} U(x,t) &= \text{total number of neutrons reflected from } x \\ &\quad \text{up to time } t \text{ due to the one trigger neutron} \\ &\quad \text{in at } x \text{ at time } t=0. \end{aligned} \tag{1}$$

Clearly,

$$U(x,t)=\int_0^t u(x,s)ds, \tag{2}$$

where u is the function of Sec. 34, now subject to the delta function type initial condition. We propose to imbed the rod of length x as usual (see Fig. 16). It should be noted that this also provides an imbedding in time, and that the important time increment is $2\Delta/c$, representing the time it takes for a particle to cross $[x, x+\Delta]$ in each direction.

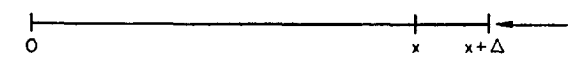

FIG. 16. Reflection from a rod of length $x+\Delta$.

We find as usual that there may be an immediate collision in $[x, x+\Delta]$, providing a flux out to the right of $\sigma\Delta$. There is also a single trigger neutron into $[0,x]$, and this enters at time $t=\Delta/c$. At time $s+\Delta/c$ let there be $u(x,s)$ neutrons/sec emergent at x. Clearly,

$$u(x,s)=(\partial U/\partial s)(x,s). \tag{3}$$

Some of these neutrons make collisions in $[x, x+\Delta]$. There is surely a flux out of $x+\Delta$ of rate $u(x,s)$. However, half of the fission neutrons return to x at this time. These provide a new source into x, and will contribute to the total flux out during the remaining $t-s$ units of time. Thus

$$\begin{aligned} U\left(x, t+\frac{2\Delta}{c}\right) &= \sigma\Delta+U(x,t) \\ &\quad +\sigma\Delta\int_0^t u(x,s)U(x, t-s)ds+0(\Delta) \end{aligned} \tag{4}$$

giving the equation of mixed differential-integral type

$$\frac{\partial U}{\partial x}+\frac{2}{c}\frac{\partial U}{\partial t}=\sigma+\sigma\int_0^t u(x,s)U(x, t-s)ds, \tag{5}$$

subject to the conditions

$$U(x,0)=0, \quad U(0,t)=0. \tag{6}$$

The system (5)–(6) has been analyzed rigorously.[47] The convolution form of the integral term makes possible an explicit analytic representation of the solution when the Laplace transform is used.

36. Modification of Medium during Transport Process

In all that has gone before, we have supposed that the properties of the medium have remained unaltered by the transport process occurring within it. This is always an approximation of greater or lesser validity.

Two very interesting processes in which interaction with the medium are taken into account are the free boundary problems of hydrodynamics, and the Stefan problems of heat conduction. As a preliminary to an investigation of Stefan-type processes by invariant imbedding techniques, we wish to discuss a one-dimensional transport process in a rod whose length is changing as a function of time.

[47] G. M. Wing, J. Math. and Mech. 7, 757 (1958).

37. Physical Process and Its Mathematical Formulation

Let us consider a rod which extends from 0 to x at time $t=0$. The rod grows, or erodes, at a specified rate so that the position of the left end is given by $X_L=f(t)$, $f(0)=0$, while the right end remains fixed, $X_R=x$. (See Fig. 17.) A neutron traversing a distance Δ in the rod has, as before, probability $\sigma\Delta+0(\Delta)$ of suffering a collision with elements of the medium. In the event of a collision, which produces fission, two neutrons emerge, one moving to the left, the other to the right. No neutron can reenter the rod once having left it, and all neutrons have constant velocity c. A single neutron, the "trigger," enters the rod at x at time $t=s$. We ask for the expected total number of neutrons that emerge at the right end up to time t, denoting this quantity by $U(x,s,t)$.

It must be noted that the condition $[-f'(t)]<c$ for all t is convenient to prevent neutrons from being rather artificially "trapped" in the rod. We shall not discuss interesting problems of this nature here.

To apply the invariant imbedding method, we immerse the original process within the class of all processes indexed by $x>0$, and then express the relationship between neighboring processes. The left ends are uniformly to obey the same law, $x_L=f(t)$, as that of the original rod.

Let us now analyze the process. At time $t=s-\Delta/c$ the trigger neutron enters at $x+\Delta$, and may or may not suffer a collision in passing from $x+\Delta$ to x. If it does, a single neutron immediately emerges at the right. In either event, a neutron passes x_R at time $t=s$. This acts as a trigger for the original rod, and produces a flux emergent from x_R at times $t>s$. The expected rate of emergence of such neutrons is given by $u(x,s,t)=(\partial U/\partial t)(x,s,t)$. Neutrons in this flux may or may not suffer collisions with the rod material in going from x to $x+\Delta$. In either event $U(x,s,t)$ neutrons emerge from $x+\Delta$ by time $t+\Delta/c$. In addition, those neutrons which do make collisions in $(x, x+\Delta)$ at time t', $s<t'<t+\Delta/c$, contribute trigger neutrons at X_R at a rate $\sigma\Delta u(x,s,t')+0(\Delta)$. The resultant flux out of $x+\Delta$ up to time $t+\Delta/c$ is then $\sigma\Delta\int_s^t u(x,s,t')U(x,t',t)dt'+0(\Delta)$. All other processes yield contributions of order $0(\Delta)$. Thus we find

$$U\left(x+\Delta, s-\frac{\Delta}{c}, t+\frac{\Delta}{c}\right)$$

$$=\sigma\Delta+U(x,s,t)+\sigma\Delta\int_s^t u(x,s,t')U(x,t',t)dt'+0(\Delta). \quad (1)$$

Hence, letting $\Delta\to 0$, we obtain the equation

$$\frac{\partial U}{\partial x}-\frac{1}{c}\frac{\partial U}{\partial s}+\frac{1}{c}\frac{\partial U}{\partial t}=\sigma+\sigma\int_s^t u(x,s,t')U(x,t',t)dt'. \quad (2)$$

The conditions imposed on U are

$$\begin{aligned} &U(x,s,t)=0, \quad s\geq t; \\ &U(x,s,t)=0, \quad f(s)=X_R. \end{aligned} \quad (3)$$

The first merely states that no neutrons emerge by time t if the trigger enters at a later time, while the second reflects the fact that none can emerge to the right if the rod is of length zero when the trigger neutron impinges.

38. Discussion

Equation (37.2) has the same general structure as that studied in our earlier sections for the case of the rod of fixed length with the neutron entering at $t=0$. It is not difficult to reduce (37.2) to the simpler equation when $f(t)=0$. However, the fact that the integral term in (37.2) is no longer of convolution form introduces new complications in studying properties of the solution.

III. DIFFUSION THEORY—A LIMITING CASE OF TRANSPORT THEORY

39. Diffusion as a Limiting Process

In previous sections in this paper, we have investigated a variety of simple models of transport theory by means of the functional equation technique of invariant imbedding. Neutrons are mathematically abstracted to be point particles with finite velocities, while fission and scattering are characterized by certain probabilities (cross sections) of branching and reversal or reorientation of direction in the medium within which the process is occurring. In the great proportion of cases we assume no neutron-neutron interaction, and no change in the properties of the medium over time, although we have discussed both of these phenomena to slight extents, Secs. 29 and 37.

It is of interest for several reasons, from both the mathematical and physical points of view, to discuss in detail what happens to the various categories of transport equations derived from different applications of invariant imbedding as the velocity of the neutron is allowed to become arbitrarily large with a corresponding increase in the probability of a collision.

This idea is a quite natural one and one that has been pursued by a number of different investigators with different aims in mind. Diffusion theory classically has been regarded as an approximation to the more rigorous

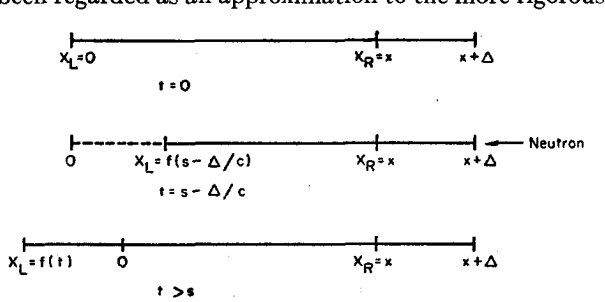

FIG. 17. Neutron transport in a rod of varying length.

(but not completely rigorous) transport theory under the assumption of high velocity and small mean free path.[48] Furthermore, passage to the limit in the "telegrapher's equation," a linear partial differential equation of hyperbolic type, has been carried out.

From another direction, the discrete random walk process yields the diffusion equation in the limit. This observation has been made the basis for a considerable amount of analytic and computational effort, centering about the theme of "Monte Carlo" techniques.

Our principal aim here is to study the limits of the nonlinear functional equations obtained from the transport processes with finite velocity, e.g., those appearing in Secs. 34 and 35, as the velocity increases without bound. In this way, we obtain corresponding results for heat or diffusion processes, where the physical picture is not as clear. Having obtained the equations in this indirect and complex fashion, we can then interpret them in such a way as to be able to derive them directly by invariant imbedding techniques. In all cases, the equations are of the generalized Riccati type which we recognize as characteristic of these processes of mathematical physics, when described in invariant imbedding.

At the present time, we are studying the question of treating Stefan-type diffusion problems by a similar passage to the limit in the equations derived from transport processes with variable boundaries. This is, as might be expected, a complex problem. Some initial results have been given in the foregoing, Sec. 37.

Throughout the sections that follow, we shall use a simple generalization of the idealized one-dimensional rod process treated in the foregoing pages. In the following section, we shall obtain some new equations for the flux within the rod, assuming finite velocities initially. In Sec. 41, we derive Fick's law for this simple process. This is important for our purposes, since it is the analysis of this result which suggests the combinations of functions which should be used in the limiting case. In Sec. 42, we study the limiting form of the internal flux as the velocity becomes infinite, and in Sec. 43 the diffusion process giving rise to the function obtained in this way is analyzed.

We then turn to our primary objective, the passage to the limit of the nonlinear integro-differential equation obtained for the reflected flux in the neutron transport case by means of the technique of invariant imbedding. In Sec. 45, we show how to obtain the result by direct application of the imbedding technique to the diffusion process.

Throughout this part of the paper, our methods are again largely formal, since we are principally interested in demonstrating the applicability of invariance principles. The existence of relevant limits and the applicability of Laplace transform methods are taken for granted in order to arrive quickly at the desired equations. These questions can be studied in a rigorous fashion, and for the simple mathematical models considered here, there is little difficulty in carrying out this program. Since, however, we know that the passage to the limit involves a reduction from a hyperbolic partial differential equation to a parabolic partial differential equation, involving *inter alia* a redundancy in the initial conditions, we can expect some difficulties in the general case. The corresponding study for ordinary differential equations when a limiting value of a parameter results in a drastic change in the order of the equation is of some subtlety. Particularly interesting examples of equations of this nature occur in various hydrodynamical investigations where viscosity plays the role of the parameter which approaches zero; cf. Wasow.[49]

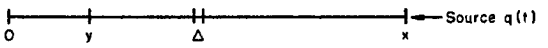

FIG. 18. The physical situation.

40. Transport Equation

To begin our work it is necessary to write down some transport equations in fairly general form. While some of them are not to be found in the literature, they may be readily derived by the methods of previous sections.

Consider a rod of material which transports neutrons, and let the neutrons have constant velocity c (monoenergetic case). The usual collision processes take place with the probability of a collision in a length Δ of the rod taken to be $\sigma\Delta+0(\Delta)$, where σ is a constant. On the average, $2k$ neutrons emerge from a collision inside the rod, k going to the left and k going to the right. We take the rod to extend from 0 to x (see Fig. 18), and designate the coordinate of an interior point by y. To initiate the process, we suppose that there is a time-dependent source, $q(t)$ neutrons incident to the left per second at x, and none at the end 0. Finally, we suppose that particles emergent at 0 or x cannot reenter the rod.

We write

$$\begin{aligned} u(y,t) &= \text{the average number of neutrons/sec passing } y \text{ at time } t \text{ and moving to the right,} \\ v(y,t) &= \text{the average number of neutrons/sec passing } y \text{ at time } t \text{ and moving to the left.} \end{aligned} \tag{1}$$

Upon using the methods outlined in Sec. 34, it is easily found that

$$\begin{gathered} (\partial u/\partial y)+(1/c)(\partial u/\partial t)=\sigma(k-1)u+\sigma kv, \\ -(\partial v/\partial y)+(1/c)(\partial v/\partial t)=\sigma ku+\sigma(k-1)v, \\ u(0,t)=0, \quad v(x,t)=q(t), \quad t\geq 0; \\ u(y,0)=v(y,0)=0, \quad 0\leq y<x. \end{gathered} \tag{2}$$

For some purposes it is convenient to talk about the total flux from time 0 to t. We shall consistently use

[48] A. Weinberg and E. Wigner, *The Physical Theory of Neutron Chain Reactors* (University of Chicago Press, Chicago, Illinois, 1958).

[49] W. Wasow, Ann. Math. **52**, 350 (1950).

capital letters to indicate quantities integrated over time. Thus

$$U(y,t)=\int_0^t u(y,z)dz,$$
$$Q(t)=\int_0^t q(z)dz, \tag{3}$$

etc. It is easy to see that the integrated quantities satisfy equations identical to (2) with the lower case letters being replaced by capitals.

At times it will be desirable to make clear the type of source in the particular problem under discussion. Hence we shall occasionally write

$$u(y,t;q),$$
$$U(y,t;q), \tag{4}$$

etc., to emphasize the source in question. The source will be deleted when the meaning is clear. In these cases we shall write $u(y,t;q)\equiv u(y,t)$, and so on. In other instances the source may be indicated and the dependence upon y or t left out.

Consider now the case in which the source consists of a single "trigger" neutron at $t=0$. Thus, formally, $q(t)=\delta(t)$, where δ is the Dirac delta function. We focus attention on the particles reflected from the rod at x, writing $r(x,t;\delta)$ for the number emergent/sec, and $R(x,t,\delta)$ for the total number emergent up to time t. Clearly,

$$r(x,t;\delta)=u(x,t;\delta),$$
$$R(x,t;\delta)=U(x,t;\delta). \tag{5}$$

However, it is again well to regard the x in the arguments of r and R as referring to the *length* of the rod rather than to the coordinates of the end point of the rod. With this rather subtle distinction in mind one then finds, proceeding as before (Sec. 35),

$$\frac{\partial R(\delta)}{\partial x}+\frac{2}{c}\frac{\partial R(\delta)}{\partial t}=\sigma k+2\sigma(k-1)R(\delta)+\sigma k\int_0^t r(x,z;\delta)R(x,t-z;\delta)dz,$$
$$R(x,0;\delta)=R(0,t;\delta)=0. \tag{6}$$

Notice that this characterizes the reflected flux in a fashion *independent of the internal fluxes*.

For the corresponding case in which there is a source $q(t)$, we note that the fundamental physical process is additive, as a consequence of our tacit assumption that there are no interactions between neutrons passing in opposite directions, we can write

$$R(x,t;q)=\int_0^t q(z)R(x,t-z;\delta)dz. \tag{7}$$

To find an equation satisfied by $R(x,t;q)$, we utilize the Laplace transform, writing

$$R(x,s)=\int_0^\infty e^{-st}R(x,t)dt, \tag{8}$$

with a consistently similar notation for transforms of other functions. Then, from (6), with $q=\delta$,

$$\frac{dR_L(\delta)}{dx}+\frac{2}{c}sR_L(\delta)=\frac{\sigma k}{s}+2\sigma(k-1)R_L(\delta)+\sigma ksR_L^2(\delta),$$
$$R_L(0,s;\delta)=0. \tag{9}$$

From (7),

$$R_L(x,s;q)=q_L(s)R_L(x,s;\delta). \tag{10}$$

Hence,

$$\frac{dR_L(q)}{dx}+\frac{2}{c}sR_L(q)=\frac{\sigma k}{s}q_L+2\sigma(R-1)R_L(q)+\sigma ksR_L(q)R_L(\delta), \tag{11}$$

which leads back to

$$\frac{\partial R(q)}{\partial x}+\frac{2}{c}\frac{\partial R(q)}{\partial t}=\sigma kQ(t)+2\sigma(k-1)R(q)+\sigma k\int_0^t r(x,z;\delta)R(x,t-z;q)dz,$$
$$R(0,t;q)=R(x,0;q)=0. \tag{12}$$

This clearly reduces to (6) when $q(t)=\delta(t)$.

We shall derive one other special case of (12), corresponding to the case when $q(t)=1$. While conceptually this may be a bit more difficult to consider than the single-trigger neutron case, it has the mathematical advantage of avoiding the δ function. For this type of source we write the integrated flux as $R(x,t;1)$ or $R(1)$ and (12) becomes

$$\frac{\partial R(1)}{\partial x}+\frac{2}{c}\frac{\partial R(1)}{\partial t}=\sigma kt+2\sigma(k-1)R(1)+\sigma k\int_0^t r(x,z;\delta)R(x,t-z;1)dz. \tag{13}$$

But, from (7),

$$R(x,t;1)=\int_0^t R(x,t-z;\delta)dz. \tag{14}$$

Then we easily find

$$\frac{\partial R(1)}{\partial x}+\frac{2}{c}\frac{\partial R(1)}{\partial t}=\sigma kt+2\sigma(k-1)R(1)+\sigma k\int_0^t r(x,z;1)r(x,t-z;1)dz,$$
$$R(0,t;1)=R(x,0;1)=0. \tag{15}$$

41. Fick's Law

If we subtract the second equation of (40.2) from the first, we obtain

$$(\partial/\partial y)(u+v)+(1/c)(\partial/\partial t)(u-v)=-\sigma(u-v). \quad (1)$$

For large c, we expect the second term on the left to be small. Hence we formally obtain the relation

$$(\partial/\partial y)(u+v)=-\sigma(u-v) \quad (2)$$

in the "limit of large velocity." Equation (2) is ordinarily referred to as *Fick's Law*,[48] which states that the net flux is proportional to the gradient of the concentration and in the opposite direction.

42. Limiting Case Obtained Directly

To obtain preliminary results we take Laplace transforms of (40.2). Thus, using the notation introduced in (40.7),

$$\begin{aligned}(du_L/dy)+(s/c)u_L&=\sigma(k-1)u_L+\sigma k v_L,\\ -(dv_L/dy)+(s/c)v_L&=\sigma k u_L+\sigma(k-1)v_L,\\ u_L(0,s)=0,\quad v_L(x,s)&=q_L(s).\end{aligned} \quad (1)$$

After rather extensive but rudimentary calculations, we arrive at the relations

$$\begin{aligned}u_L(y,s)&=\frac{k\sigma q_L(s)\sinh\lambda y}{\{\lambda\cosh\lambda x+[(s/c)+(1-k)\sigma]\sinh\lambda x\}},\\ v_L(y,s)&=\frac{q_L(s)\{\lambda\cosh\lambda y+[(s/c)+(1-k)\sigma]\sinh\lambda y\}}{\{\lambda\cosh\lambda x+[(s/c)+(1-k)\sigma]\sinh\lambda x\}},\end{aligned} \quad (2)$$

where

$$\lambda^2=(s/c)^2+[2(1-k)\sigma/c]s+\sigma^2(1-2k). \quad (3)$$

We now choose $k=\frac{1}{2}$, which means physically that an average collision gives rise to one neutron. This choice eliminates the last term in (3). Since we seek a diffusion type equation, we let $c\to\infty$, which is to say, we allow the velocity to become infinite. Clearly, to preserve the process we must then require that $\sigma\to\infty$ in such a way that $\lim c/\sigma=D$, a constant. Hence, from what has proceeded, $\lim\lambda=(s/D)^{\frac{1}{2}}$.

(It should be noted that a somewhat more general result could have been obtained by requiring, instead of $k=\frac{1}{2}$, that $\lim\sigma^2(1-2k)=\alpha$. By so doing we could have accounted for cases of absorption or fission. To do this here would merely complicate the ensuing calculations.)

Bearing (50.2) in mind, we set

$$\begin{aligned}j_L(y,s)&=\sigma[u_L(y,s)-v_L(y,s)],\\ j_{0,L}(y,s)&=\lim_{\sigma\to\infty}j_L(y,s).\end{aligned} \quad (4)$$

Let us consistently reserve the subscript zero to refer to quantities in the limit as $c\to\infty$.

We then discover that

$$\begin{aligned}j_{0,L}(y,s)&=-\lim_{\sigma\to\infty}\frac{\sigma q_L(s)\lambda\cosh\lambda y}{\{\lambda\cosh\lambda x+[(s/c)+(\sigma/2)]\sinh\lambda x\}}\\ &=-2q_L(s)\frac{(D^{-1}s)^{\frac{1}{2}}\cosh[y(D^{-1}s)^{\frac{1}{2}}]}{\sinh[x(D^{-1}s)^{\frac{1}{2}}]}.\end{aligned} \quad (5)$$

43. Classical Diffusion Problem

We now seek an ordinary diffusion problem which gives rise to the limiting expression found in (41.5). It is readily verified that if $\theta(y,t)$ is implicitly determined by the relations

$$D\frac{\partial^2\theta}{\partial y^2}=\frac{\partial\theta}{\partial t},\quad \theta(0,t)=0,\quad \theta(x,t)=2q(t),\quad \theta(y,0)=0, \quad (1)$$

then, explicitly,

$$\theta_L(y,s)=\frac{2q_L(s)\sinh[y(D^{-1}s)^{\frac{1}{2}}]}{\sinh[x(D^{-1}s)^{\frac{1}{2}}]}, \quad (2)$$

and

$$\frac{d\theta_L}{dy}=2q_L(s)(D^{-1}s)^{\frac{1}{2}}\frac{\cosh[y(D^{-1}s)^{\frac{1}{2}}]}{\sinh[x(D^{-1}s)^{\frac{1}{2}}]}. \quad (3)$$

We may summarize our results thus far as follows:

If we consider the transport problem formulated in (40.2) in the limiting case where $c\to\infty$, $c/\sigma\to D$, with $k=\frac{1}{2}$, then the problem is formally equivalent to the classical diffusion problem (1). The quantity

$$\lim_{\sigma\to\infty}[u(y,t)+v(y,t)]$$

may be identified with $\theta(y,t)$, while

$$\lim_{\sigma\to\infty}\sigma[u(y,t)-v(y,t)]$$

corresponds to $-\partial\theta/\partial y$.

It is possible to identify $\theta(y,t)$ with the total neutron flux [see (40)] although the diffusion may refer as well to heat or material concentration. The fact that a source of $2q(t)$ is required as part of the initial conditions in the problem (1) may be rather puzzling until one notes from (42.2) that, formally, both $u(x,t)$ and $v(x,t)$ approach $q(t)$ as $c\to\infty$.

44. Reflected Flux

Let us now turn to Eq. (40.15) and try to carry out the same type of passage to the limit. It is clear that we must begin by investigating the quantity

$$H(x,t;q)=\sigma\{R(x,t;q)-Q(t)\}, \quad (1)$$

which reduces to $\sigma\{R(x,t;1)-t\}$, when $q(t)=1$. Thus,

$$\begin{aligned}R(1)&=[H(1)/\sigma]+t,\\ r(1)&=[h(1)/\sigma]+1.\end{aligned} \quad (2)$$

If we substitute these in (40.15) with $k=\frac{1}{2}$, we find

$$\frac{1}{\sigma}\frac{\partial H(1)}{\partial x}+\frac{2}{c}\left(\frac{h(1)}{\sigma}+1\right)$$
$$=\frac{\sigma t}{2}-\sigma\left(\frac{H(1)}{\sigma}+t\right)+\frac{\sigma}{2}\int_0^t\left\{\frac{h(x,z;1)}{\sigma}+1\right\}$$
$$\times\left\{\frac{h(x,t-z;1)}{\sigma}+1\right\}dz. \quad (3)$$

From this we readily obtain

$$\frac{\partial H(1)}{\partial x}+\frac{2\sigma}{c}\left(\frac{h(1)}{\sigma}+1\right)=\frac{1}{2}\int_0^t h(x,z;1)h(x,t-z;1),$$
$$H(x,0;1)=0, \quad H(0,t;1)=-\sigma t. \quad (4)$$

On passing to the limit as in Sec. 43, we obtain (at least formally)

$$\frac{\partial H_0(1)}{\partial x}+2D^{-1}=\frac{1}{2}\int_0^t h_0(x,z;1)h_0(x,t-z;1)dz,$$
$$H_0(x,0;1)=0, \quad H_0(0,t;1)=-\infty; \quad (5)$$

where $H_0(x,t;q)=\lim_{\sigma\to\infty}H(x,t;q)$, etc., as agreed. That (5) is the correct limiting form may be established by a Laplace transform argument similar to that of the last section. We omit the details.

It is of some interest to evaluate H_0. This may be done by solving (5). However, it is easier for us to note from (42.5) that

$$h_{0,L}(x,s;q)=-2q_L(s)\frac{(D^{-1}s)^{\frac{1}{2}}\cosh[x(D^{-1}s)^{\frac{1}{2}}]}{\sinh[x(D^{-1}s)^{\frac{1}{2}}]}$$
$$=-[2/(sD)^{\frac{1}{2}}]\coth[x(D^{-1}s)^{\frac{1}{2}}], \quad (6)$$

when $q(t)=1$. We find

$$h_0(x,t;1)=-\frac{2}{(\pi tD)^{\frac{1}{2}}}\left\{1+2\sum_{n=1}^{\infty}\exp\left(-\frac{x^2n^2}{tD}\right)\right\}$$
$$=-\frac{2}{x}\theta_0\left(\frac{1}{2},\frac{t}{Dx^2}\right), \quad (7)$$

where θ_0 is a theta function.

The analog of (5) may be derived easily for the case in which there is an arbitrary source $Q(t)$. The result is

$$\frac{\partial H_0(q)}{\partial x}+2D^{-1}q(t)=\frac{1}{2}\int_0^t h_0(x,z;1)h_0(x,t-z;q)dz,$$
$$H_0(x,0;q)=0, \quad H_0(0,t;q)=-\infty. \quad (8)$$

We now readily see the following result:

If we consider the transport problem formulated in (40.2) in the limiting case then the quantity $H_0(x,t;q)$ is formally equivalent to the quantity $-(\partial/\partial y)\int_0^t\theta(y,z)dz|_{y=x}$ where θ is defined by (43.1). Further, $H_0(q)$ satisfies (8) with $h_0(1)$ given by (5).

45. Direct Invariant Imbedding Approach in Diffusion Theory

The equations thus far obtained are not new, though our approach to them may be somewhat novel. To conclude our work here we shall present a method of obtaining (44.8) by invariant imbedding techniques without venturing outside the confines of ordinary diffusion theory. The method described holds promise of being applicable in much more complicated diffusion processes than that described here, and, in particular, may eventually yield new formulations of Stefan-type problems.

To be consistent in our viewpoint, we now think of $\phi(y,t)$ as the density of neutrons at y at time t. Then the net neutron current density $i(y,t)$ is provided by Fick's Law, in the ordinary diffusion approach,[48]

$$i(y,t)=-D(\partial/\partial y)\phi(y,t). \quad (1)$$

The conservation of particles (since there is no internal production when $k=\frac{1}{2}$) requires in any interval (a,b) of the rod

$$i(b,t)-i(a,t)=-\frac{\partial}{\partial t}\int_a^b\phi(y,t)dy. \quad (2)$$

Let us write, for the net current emerging from our rod of length x, $k(x,t)$. Here, again, while it is true that $k(x,t)=i(x,t)$ we choose to regard the x in the function k as referring to the *length* of the rod. Thus $k(x+\Delta,t)$ is the net current emergent from a rod of length $x+\Delta$, source $2q(t)$ at $(x+\Delta)$, other initial and boundary conditions being as before.

We now try to express $k(x+\Delta,t)$ in terms of $k(x,t)$. Upon applying (2) to the rod of length $x+\Delta$, we find

$$k(x+\Delta,t)-i(x,t)=-\frac{\partial}{\partial t}\int_x^{x+\Delta}\phi(y,t)dy, \quad (3)$$

or, integrating over time,

$$K(x+\Delta,t)-I(x,t)=-\int_x^{x+\Delta}\phi(y,t)dy. \quad (4)$$

We now seek expressions for $I(x,t)$ and ϕ. To find $I(x,t)$ we note that we have thus far disregarded the part of the rod from 0 to x. By the continuity conditions imposed by diffusion theory, we know that $I(x,t)$ is merely the current out of x due to the source $\phi(x,t)$ imposed. Let us suppose that a steady source of unit strength produces a current out of the rod of $p(x,t)$. Then a source (x,t) will produce an integrated current

$$I(x,t)=\int_0^t p(x,t-z)\phi(x,z)dz. \quad (5)$$

(This is just Duhamel's principle.[46])

As yet we have not used (1). From it we find

$$\phi(x,t)=(\Delta/D)k(x+\Delta,t)+2q(t)+0(\Delta). \tag{6}$$

On substituting (5) and (6) in (4), we obtain

$$K(x+\Delta,t)=\int_0^t p(x,t-z)\left\{\frac{\Delta}{D}k(x+\Delta,z)+2q(z)\right\}dz - 2\Delta q(t)+0(\Delta). \tag{7}$$

But, by Duhamel's principle,

$$\int_0^t p(x,t-z)2q(z)dz=K(x,t). \tag{8}$$

Thus

$$\frac{\partial K}{\partial x}+2q(t)=\frac{1}{D}\int_0^t p(x,t-z)k(x,z)dz. \tag{9}$$

This agrees with (44.8) upon identifying k with $Dh_0(q)$ and p with $(D/2)h_0(1)$, the factor $\frac{1}{2}$ occurring because p is the current due to a unit source, while h_0 is obtained from a source of strength 2.

It is clear that

$$K(x,0)=0. \tag{10}$$

To find $K(0,t)$ we note from (6) that

$$\phi(0,t)=0=(\Delta/D)k(\Delta,t)+2q(t)+0(\Delta),$$

so that for $Q(t)>0$,

$$K(0,t)=-\infty. \tag{11}$$

Clearly, in case $q=1$, we have

$$\frac{\partial P}{\partial x}+2=\frac{1}{D}\int_0^t p(x,t-z)p(x,z)dz,$$

$$P(x,0)=0, \quad P(0,t)=-\infty. \tag{12}$$

IV. RANDOM WALK AND MULTIPLE SCATTERING

46. Random Walk

We now wish to apply invariant imbedding techniques to the study of random walk processes. Subsequently, we shall consider more general processes of this nature, equivalent to multiple scattering processes.

Consider the finite one-dimensional lattice consisting of the integer values between a and b along the real line, as indicated in Fig. 19. A particle jumps from lattice-point to lattice-point in accordance with the following law. When at k, there is a probability $q(k)$ of moving one unit to the right and a probability $p(k)=1-q(k)$ of moving one unit to the left.

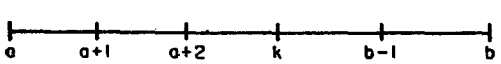

FIG. 19. A one-dimensional lattice.

We wish to determine the probability, that the particle starting at k, hits the barrier at a before it hits the barrier at b. The process ends as soon as the particle lands at a or b—hence, the name "*absorbing barriers.*"

This is an extension of the classical "gambler's ruin" process in which $p(k)=q(k)=\frac{1}{2}$ for $a<k<b$. This particular case can be treated in a very elegant fashion by means of Wald's "fundamental identity." See Bellman for generalizations to the case of dependent steps.[50] Another extension is the "game of survival."[20]

The classical approach, also based upon the use of recurrence relations, proceeds as follows[51]:

Let

$u(k)=$ the probability that a particle starting at k lands at a before it lands at b. (1)

Then, considering what happens as a result of the first step, for $a<k<b$,

$$u(k)=p(k)u(k-1)+q(k)u(k+1), \tag{2}$$

with the two-point boundary conditions

$$u(a)=1, \quad u(b)=0. \tag{3}$$

We thus face the problem of solving a system of linear equations, something we wish to avoid if possible. In what follows we shall attack these problems by a quite different method.

47. Invariant Imbedding Approach

The observation that the desired probability $u(k)$ is a function of the endpoints a and b, as well as of k, keys our approach. Hence, we should write $u(k,a,b)$ to signify this dependence.

Invariant imbedding, as we have repeatedly stated, capitalizes upon this dependence. In place of considering a and b to be constants, we consider them to be parameters of equal importance with k, which means that in place of treating an individual random walk process, we investigate simultaneously an entire family of processes. The individual problem is then analyzed in terms of its relation to contiguous members of the family. In this way, we hope to construct a bridge between particular elements of the family of quite simple analytic structure and the processes of interest to us.

Let us then keep one endpoint fixed, say b, and regard u as a function of a and k. To make this dependence explicit, let us introduce the new function

$f(a,k)=$ the probability that a particle starting at k, $a\leq k\leq b$, will reach a before reaching b. (1)

Clearly, $f(a,k)=u(k;a,b)$.

To obtain the required relation between contiguous elements, we use the simple geometric fact that a particle starting at k, and moving one unit in either direc-

[50] R. Bellman, Proc. Cambridge Phil. Soc. **53**, 257 (1957).
[51] S. Chandrasekhar, Revs. Modern Phys. **15**, 1 (1943).

tion at each stage, must hit $a+1$ before it can hit a. This is analogous to the stratification technique we used in the discussion of neutron transport and multiplication. On having reached $a+1$, the particle must then reach a before b, if this is to be the case for the original process.

On translating these remarks into algebraic relations, and using the elementary rules of probability theory, we have

$$f(a,k)=f(a+1,k)f(a,a+1). \tag{2}$$

Upon iterating this relation, we have

$$f(a,k)=f(a,a+1)f(a+1,a+2)\cdots f(k-1,k). \tag{3}$$

an interesting representation for solutions of a Jacobi system of equations of the type appearing in (37.2).

We have deliberately stressed the word "elementary" in the foregoing discussion, since we can employ similar methods based upon other concepts of probability to discuss other kinds of equations. For other methods of treating Jacobi equations, see Bellman.[52]

48. Function $f(a, a+1)$

To answer our original question, that of determining the value of $f(a,k)$, it remains to evaluate the functions of one variable

$$g(a)=f(a,a+1), \tag{1}$$

defined for $a\leq b-1$. Clearly, $g(b-1)=0$.

If we revert to the description of the original process, we obtain the relation

$$f(a,a+1)=p(a+1)+q(a+1)f(a,a+2). \tag{2}$$

If we use (47.2), we have

$$f(a,a+2)=f(a+1,a+2)f(a,a+1). \tag{3}$$

If we combine these two expressions, we obtain the recurrence relation

$$g(a)=p(a+1)/[1-q(a+1)g(a+1)]. \tag{4}$$

Since, as noted in the foregoing, $g(b-1)=0$, we have a simple inductive determination of $u(a)$ for $a\leq b-1$.

49. An Alternative Derivation

The foregoing result can be derived in a way which emphasizes its physical significance and its connection with previous work on neutron diffusion. Toward this end, let us consider the following scattering problem. A rod extending from a to b has the property that if a particle is at the position k, there is probability $p(k)$ that it will be scattered to $k-1$, and probability $q(k)=1-p(k)$ that it will be scattered to $k+1$. A particle is placed at the end a, and we wish to determine the probability that it will be "back-scattered" (reflected) from a, over all time, rather than be "forward-scattered" (transmitted) through the end b.

We imbed this process within the class of processes with "trigger" particles placed at the end l of rods extending from l to b, with $l=b, b-1, \cdots$, and then write a functional equation interconnecting these processes.

Let us define the function $g(a)$ directly

$g(a)=$ the probability that over all time a particle at $a+1$ will be backscattered to a by the rod extending from $a+1$ to b, rather than be forwardscattered at b from the rod. (1)

Observe next that with the particle initially at the position $a+1$, there is probability $p(a+1)$ that it will be scattered directly to the point a. On the other hand, if it is scattered initially to the right to $(a+2)$, then by definition there is probability $g(a+1)$ that it will eventually be back-scattered from the rod $(a+2, b)$ to the point $a+1$, from which it may be scattered to the point a. Should, however, it once again be scattered to the right, to the point $(a+2)$, there is once again probability $g(a+1)$ that it will eventually reach the point $a+1$, and so on. In this way we see that

$$g(a)=p(a+1)+q(a+1)g(a+1)p(a+1)+q(a+1)\times g(a+1)q(a+1)g(a+1)p(a+1)+\cdots, \tag{2}$$

which, upon summing the geometric series on the right hand side, leads to the equation

$$g(a)=p(a+1)/[1-q(a+1)g(a+1)]. \tag{3}$$

This is Eq. (48.4).

The method that we have used in deriving Eq. (48.2) of (3) corresponds abstractly to the method used by Ambarzumian[6] in discussing diffuse reflection from a foggy medium, a process we shall discuss later, and to the method used above in handling some neutron transport processes.

Similarly, the discussion in Sec. 47 may be reinterpreted to yield the flux scattered from the end a of a rod as a result of an internal source of particles.

50. Expected Sojourn

Let us now introduce the function

$w(a,k)=$ the conditional expected time required for the particle to reach a before reaching b, starting from k, assuming a unit step takes unit time. (1)

By this we mean the expected time required to reach a, under the assumption that a is reached before b. Then, the same foregoing reasoning yields the relation

$$w(a,k)=w(a+1,k)+w(a,a+1). \tag{2}$$

To obtain an analytic expression for $w(a,a+1)$, we

[52] R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill Book Company, Inc., New York, 1960).

combine the two expressions

$$w(a, a+1)=p(a+1)+q(a+1)[w(a, a+2)+1], \qquad w(a, a+2)=w(a+1, a+2)+w(a, a+1). \tag{3}$$

The result is

$$w(a, a+1)=\frac{1}{p(a+1)}+\frac{q(a+1)}{p(a+1)}w(a+1, a+2). \tag{4}$$

Iteration yields the infinite series

$$w(a, a+1)=\frac{1}{p(a+1)}+\frac{q(a+1)}{p(a+2)p(a+1)}+\frac{q(a+1)q(a+2)}{p(a+3)p(a+2)p(a+1)}+\cdots, \tag{5}$$

with the convention that the series terminates if b is finite.

51. Characteristic Functions

As we have pointed out in the foregoing, whenever an expected value can be determined, the same techniques yield relations for generating functions. Let

$$y(a,k,s)=E(e^{isz}), \tag{1}$$

where $z=z(a,k)$ is the random variable equal to the time spent by the particle in going from k to a, without ever hitting b.

Since

$$z(a,k)=z(a+1, k)+z(a, a+1), \tag{2}$$

we have the functional equation

$$y(a,k,s)=y(a+1, k, s)y(a, a+1, s). \tag{3}$$

It is now not hard to show that

$$y(a, a+1)=p(a+1)e^{is}+q(a+1)e^{is}y(a, a+2), \qquad y(a, a+2)=y(a+1, a+2)y(a, a+1). \tag{4}$$

From these we obtain the recurrence relation

$$y(a, a+1)=p(a+1)e^{is}/[1-q(a+1)e^{is}y(a+1, a+2)], \tag{5}$$

which can be used to obtain higher moments.[53]

52. More General Random Walk Processes

Similar methods can be applied to random walks which allow steps of different units at each stage. Abstractly, these methods will be equivalent when vector-matrix notation is introduced.

53. Multiple Scattering

In this section, we wish to consider two processes of particular interest. The first concerns a one-dimensional random walk in which the energy of the particle changes as a result of its wandering, while the second pertains to a two- or-three-dimensional random walk process in which the direction of motion changes as a result of each collision.

Both of these can, in discrete form, be considered to be particular cases of a process of the following type: "A particle in state i, $i=1, 2, \cdots, N$, can occupy any of the lattice points k between a and b. Let

$$p_{ij}(k)=\text{the probability that a particle at } k \text{ in state } i \text{ will go one unit to the left, and arrive in state } j,\ i,\ j=1, 2, \cdots, N,$$
$$q_{ij}(k)=\text{the probability that a particle at } k \text{ in state } i \text{ will go one unit to the right, and arrive in state } j,\ i,\ j=1, 2, \cdots, N." \tag{1}$$[54]

Let us then define the N^2 functions

$$u_{ij}(a,k)=\text{the probability that a particle starting at } k \text{ in state } i \text{ will hit } a \text{ in states } j \text{ before reaching } b \text{ in any state.} \tag{2}$$

Proceeding as in the foregoing sections, we obtain the relation

$$u_{ij}(a,k)=\sum_m u_{im}(a+1, k)u_{mj}(a, a+1). \tag{3}$$

Consequently, if we introduce the matrix function

$$U(a,k)=[u_{ij}(a,k)], \tag{4}$$

we derive the basic relation

$$U(a,k)=U(a+1, k)U(a, a+1), \tag{5}$$

the analog of (47.2). Once again, we see that the problem has reduced to a determination of a function of a alone, $U(a, a+1)$.

54. Determination of $U(a, a+1)$

Proceeding as before, we have

$$u_{ij}(a, a+1)=p_{ij}(a+1)+\sum_m q_{im}(a+1)u_{mj}(a, a+2), \tag{1}$$

or, if $G(a)=[u_{ij}(a, a+1)]$, $P(a)=[p_{ij}(a)]$, $Q(a)=[q_{ij}(a)]$,

$$G(a)=P(a+1)+Q(a+1)U(a, a+2). \tag{2}$$

If we use (53.2), we obtain the relation

$$U(a, a+2)=U(a+1, a+2)U(a, a+1). \tag{3}$$

If we use this in (2), we have

$$G(a)=P(a+1)+Q(a+1)G(a+1)G(a), \tag{4}$$

or

$$G(a)=[I-Q(a+1)G(a+1)]^{-1}P(a+1). \tag{5}$$

Since $G(b-1)=0$, once again we have a direct iterative technique for determining $G(a)$, and thus $U(a,x)$.

[53] R. Bellman and R. Kalaba, J. Math. and Mech. 9, 411 (1960).

[54] It is convenient here to reverse the index order as compared to previous usage (see Sec. 8).

55. Discussion

It is clear that in the same way we can obtain multidimensional analogs of the results for the expected sojourn and generating function.

Turning from the analytic aspects, let us examine the computational aspects. Approaching the problem along conventional lines, we obtain a system of linear equations of the form

$$u_{ij}(k)=\sum_m p_{im}u_{mj}(k-1)+\sum_m q_{im}(k)u_{mj}(k+1). \quad (1)$$

On keeping j fixed, we have a system of order $N(b-a)$. If $N=10$, and $b-a=100$, this is order 1000, a respectable and even formidable number, even in the light of modern devices.

On using the technique described in the foregoing, the solution is made to depend upon the inversion and repeated multiplication of 10×10 matrices, a complicated, but far more feasible process.

56. Time-Dependent Processes

Let us now consider the one-dimensional random walk process in which each stage consumes one time unit. Let

$u(a,k,t)$ = the probability of going from k to a in time t, without ever hitting b. (1)

As we shall see, we derive equations completely analogous to those exhibited in the foregoing for the generating function

$$F(a,k,t,r)\equiv F(a,k)=\sum_{t=0}^{\infty} u(a,k,t)r^t. \quad (2)$$

As in the previous sections, we obtain the fundamental relation

$$u(a,k,t)=\sum_{s=0}^{t} u(a+1,k,s)u(a,a+1,t-s), \quad (3)$$

and once again derive the fundamental relation

$$F(a,k)=F(a+1,k)F(a,a+1). \quad (4)$$

Furthermore,

$$u(a,a+1,t)=p(a+1)\delta(1,t)+q(a+1)u(a,a+2,t-1), \quad (5)$$

for $t\geq 1$, where

$$\delta(1,t)=1, \quad t=1, \qquad =0, \quad t\neq 1. \quad (6)$$

Thus, multiplying (5) by r^t and summing over t,

$$F(a,a+1)=p(a+1)r+q(a+1)rF(a,a+2). \quad (7)$$

From here on the argument proceeds as before. The final result is

$$F(a,a+1)=p(a+1)r/[1-q(a+1)rF(a+1,a+2)]. \quad (8)$$

Equation (7) can be derived directly making use of the properties of the process and of generating functions. It should be compared with (51.5).

V. RADIATIVE TRANSFER

57. Introduction

In these last few sections we shall discuss a problem arising in the field of radiative transfer. Abstractly, such cases are equivalent to appropriate neutron transport problems, and therefore the material appearing here could very well have been placed in earlier sections. However, since it was in the solution of problems of this genre that Ambarzumian[6] first successfully used his invariance principle and here, too, that Chandrasekhar developed his extensive generalization[5] it seems fitting that we leave these problems in their original setting. Our discussion follows that of[55] in which the principle of invariant imbedding was first sketched.

58. Physical Model

Assume that parallel rays of light of uniform intensity are incident on an inhomogeneous slab composed of a substance which absorbs and scatters light. Our objective is to determine the intensity of the diffusely reflected light as a function of the incident light, the properties of the slab, and the angle of the emerging rays.

We shall assume the slab has the following absorption and scattering properties:

1. In traversing a distance d in the slab a portion of a beam I is reduced to intensity $I(1-ad)+0(d)$. A fraction λ of the intercepted beam is reradiated, while a fraction $1-\lambda$ is permanently lost (absorbed). The quantities λ and a may be dependent upon the distance from an edge of the slab.
2. Radiation is scattered isotropically.

In the light of our previous work, it is most convenient to consider the light radiation as composed of photons; particles, then, which behave, for our purposes, just as neutrons do.

We must note, too, that in reality not only the angles ψ and θ (Fig. 20) arise but also the corresponding azimuthal angles. The latter may be neglected in our analysis because of the symmetry of the problem.

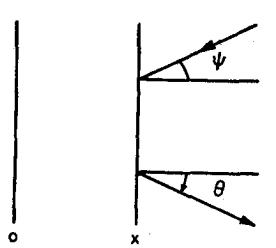

FIG. 20. Cross section of slab with incident and reflected rays.

[55] R. Bellman and R. Kalaba, Proc. Natl. Acad. Sci. U. S. 42, 629 (1956).

We define a reflection coefficient $R(x,\psi,\theta)$, giving the intensity of radiation reflected in direction θ per unit area on the face of the slab due to a beam of unit intensity incident at angle ψ, the thickness of the slab being x. Otherwise put, R is the number of photons per unit time out of a unit area on the slab at angle θ, due to a unit flux (one photon per unit area per unit time) impinging at angle ψ.

It is now easy to write down the equations for R, either using directly the fundamental principles we have developed, or applying the general flux equation (26.2). We find, recalling that integrations over the azimuthal angles are necessary, even though R is independent of them,

$$\frac{\partial R}{\partial x}=\frac{a(x)\lambda(x)}{4\pi\cos\psi}-a(x)\left(\frac{1}{\cos\theta}+\frac{1}{\cos\psi}\right)R(x,\psi,\theta)$$
$$+\frac{a(x)\lambda(x)}{2\cos\psi}\int_0^{\pi/2}R(x,\psi',\theta)\sin\psi'd\psi'$$
$$+\frac{a(x)\lambda(x)}{2}\int_0^{\pi/2}R(x,\psi,\theta')\frac{\sin\theta'}{\cos\theta'}d\theta'$$
$$+a(x)\lambda(x)\pi\int_0^{\pi/2}\frac{\sin\theta'}{\cos\theta'}R(x,\psi,\theta')d\theta'$$
$$\times\int_0^{\pi/2}R(x,\psi',\theta)\sin\psi'd\psi'. \quad (1)$$

59. Comparison with the Results of Ambarzumian

Equation (58.1) is considerably more general than the original result of Ambarzumian, since that writer considered a semi-infinite slab, with $a=1$ and λ constant. Our result should hence reduce to his when we eliminate the x dependence and set $\partial R/\partial x=0$. The reader will find, however, that the equations still differ considerably.

The reason for this apparent discrepancy lies in the way we have chosen to measure flux throughout this paper. While classically flux is measured in terms of the number of particles per unit time crossing a unit area *normal* to the direction of the particle, we have chosen instead to talk in terms of the number per unit time through a unit area on the (geometric) surface through which the particles are passing.

A bit of philosophy may be appropriate. The transport equation for the flux of particles internal to a body ordinarily is quite independent of the boundaries of the medium itself. The geometry is brought in through the auxiliary boundary conditions. Thus a person in outer space, with no frame of reference, would rather naturally measure flux in the classical way.

The equations of invariant imbedding, however, depend deeply and inherently upon the boundaries of the body under consideration. It therefore seems natural to define the flux with direct reference to those boundaries. We have found this the easier way conceptually.

In any event it is possible to convert from one definition of flux to the other without great effort. Consider the case of Sec. 58, and let us define $I(x,\psi,\theta)$ as the reflected intensity in the classical sense: $I(x,\psi,\theta)$ is the number of photons reflected from x travelling in direction θ per unit time through a unit area normal to that direction due to one photon incident on x per unit time per unit area normal to the direction ψ. Then it is easy to see that

$$I(x,\psi,\theta)=R(x,\psi,\theta)(\cos\psi/\cos\theta). \quad (1)$$

If we use the foregoing transformation, we obtain Ambarzumian's equation.

VI. SUMMARY

60. Review of Basic Techniques

Having covered some quite diverse parts of mathematical physics, we feel that it is important to state to the reader what our basic ideas and objectives have been, and what have been the methods we have employed toward obtaining these goals.

We start with the fact that any physical process can be described in a variety of different ways, leading to a number of different analytic paraphrases. As soon as this most important fact is accepted, then necessarily the premise must be accepted that some descriptions will be significantly better than others for the study of particular properties of a process.

We have hinged our description of physical processes upon the *invariance concept*. By this we mean that we have consistently introduced state variables and written our equations in such a way as to stress the idea that any individual process is to be considered as a member of a family of related processes. The advantage to be gained from this point of view resides in the common observation that the properties of a particular member of a set can often be easily understood in terms of the properties of contiguous elements, although often quite puzzling to comprehend in isolation. This principle of continuity, one of the most powerful and versatile tools in the mathematician's hopechest, is basic also in the biological world.

The usual equations of mathematical physics arise from the application of imbedding techniques, by means of the introduction of fluxes at arbitrary points, by means of the introduction of time, and so on. By introducing other parameters of significance and applying invariance principles in a different fashion, we have obtained new equations which possess certain computational and analytic advantages over the classical formulations. We have indicated how one can pass back and forth from one type of equation to the other.

One of the major difficulties of the classical approach lies in the fact that it leads to boundary value problems which in turn lead to Fredholm integral equations.

Ultimately, for the solution of these problems in numerical terms, we are forced to the solution of large systems of linear equations. This is a most subtle and difficult problem and one for which modern digital computers are not well suited.

The new approach presented here leads to the solution of initial value problems, not necessarily in time but in other meaningful physical parameters, and computationally to the iteration of nonlinear transformations. This latter is a task well designed for the digital computer. Finally, we note that our formulation very often corresponds to the way the data is obtained experimentally.

Let us note in passing that there are available other techniques for converting boundary-value problems involving Fredholm-type integral equations to initial value problems relying upon Volterra-type integral equations. Generalizing results of Holmgren and Levi, Muntz discussed how this could be done for the heat equation, while Milgram and Rosenbloom used a different device for treating generalized potential theory, involving the harmonic integrals of Hodge. Our methods are quite different from theirs, since ours always involve a variation of the domain, while theirs keep the domain fixed.

Secondly, let us point out that the Riccati equations which are characteristic of our approach can be obtained in a number of different ways in dealing with ordinary second-order differential equations. The derivation we employ is quite different from that obtained by a simple change of a dependent variable, and different also from that resulting from dynamic programming. Our methods lead naturally to the generalized Riccati equations corresponding to partial differential operators.

The functions with which we deal, the reflection and transmission functions, appear to be basic functions of analysis. This is to be expected since they represent fundamental physical quantities. If we use these functions we obtain a new approach to the problems of existence and uniqueness of solutions of the classical equations, and new representations for the solutions of these equations. What is most important is that these methods are independent of characteristic value and spectral theory. Results of this type will appear in the near future.

Although we have from time to time mentioned various computational advantages of our procedures, we have not included any calculations in this paper for several reasons. In the first place, the paper has already assumed a certain unwieldy length. Far more important is the fact that numerical solution of significant problems introduce a number of nontrivial questions, regardless of the method that is used. Any who have engaged in the computational solution of equations will sadly testify to this. Consequently, we feel that it is better to leave the calculations for a separate study, devoted merely to this aspect.

Statistical Dynamics of Simple Cubic Lattices. Model for the Study of Brownian Motion*

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The system considered is an n-dimensional cubic crystal with nearest-neighbor central and noncentral harmonic forces in which the mass M of one of the lattice particles is relatively large. It is assumed that the velocities and positions of the light particles in the system (mass m) are normally distributed, at time $t=0$, as in thermal equilibrium. The conditional velocity distribution for the heavy particle at time t is then a normal distribution with a time-dependent mean value. This mean value is the velocity autocorrelation function. The dispersion of the distribution is shown to be a simple function of the autocorrelation. In the limit $M/m \gg 1$ in the one- and two-dimensional lattices, the autocorrelation function is, respectively, a damped exponential and a damped oscillating exponential. These different types of statistical behavior are related to the different dynamic properties of the medium with which the heavy particle interacts.

I. INTRODUCTION

IN this paper we study a classical mechanical model which exhibits Brownian-like motion. The model is a modification of the simple n-dimensional cubic type crystal lattice with nearest-neighbor central and noncentral harmonic forces. There have been a considerable number of investigations of the properties of such models recently.[1-3] Therefore, it is interesting to note that the dynamical properties of the one-, two-, and three-dimensional lattices were studied extensively by Hamilton[3] in 1839. The modification of the lattice model in this paper is made by increasing the mass of one of the lattice particles to a relatively large value. The conditional velocity distribution function for the heavy particle is obtained from the solution of the equations of motion of the entire lattice. Only one statistical, or nonmechanical, element is introduced, namely, the initial positions and velocities of the particles in the crystal are assumed to be canonically distributed.[4] There is a marked contrast between the detailed microscopic treatment in this paper and the phenomenological treatments of Brownian motion which start with a Langevin or Fokker-Planck equation.[5]

In Sec. II the equations of motion of the lattice are solved, and a simple expression is obtained for the velocity of the heavy particle at time t as a linear combination of the initial positions and velocities of all the particles in the lattice. In Sec. III it is assumed that the initial positions and velocities of the light particles in the lattice are canonically (normally) distributed and that the initial velocity of the heavy particle is v_0. Under these conditions, an expression is obtained for the probability that the velocity of the heavy particle is v at time t. This expression for the conditional velocity distribution function is a gaussian distribution whose mean and standard deviation are both related to the velocity autocorrelation function. In Sec. IV explicit expressions are obtained for the velocity autocorrelation function in the case of the one- and the two-dimensional lattices. In the one-dimensional case, the known result[6] that the autocorrelation function is a simple exponential is obtained. In the two-dimensional case, the autocorrelation function is shown to be an exponentially damped, oscillating function of the time. We note that the autocorrelation functions obtained from the one- and two-dimensional lattice models have the same form as the autocorrelation functions derived from phenomenological Langevin equations for a free and for a harmonically bound particle, respectively.

II. DESCRIPTION OF MODEL AND SOLUTION OF EQUATIONS OF MOTION

We consider a modification of an n-dimensional lattice with nearest-neighbor central and noncentral harmonic forces and with periodic boundary conditions.[1] There are assumed to be $2N+1$ lattice points in each of the lattice directions, labelled from $-N$ to $+N$. A particle in the lattice is designated by the n-component vector $\mathbf{R}$ whose components r_j are integers such that $-N \leqslant r_j \leqslant N$, $j=1, \cdots, n$. The principal modification which is introduced into the conventional model is that the mass of particle $\mathbf{0}=\{0, \cdots, 0\}$ is M, whereas the

* Parts of this paper were presented at the Annual meeting of the American Physical Society (January 27-30, 1960). R. J. Rubin, Bull. Am. Phys. Soc. Ser. II, 5, 7 (1960).

[1] E. W. Montroll, *Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability* (University of California Press, Berkeley, California, 1956), Vol. 3, p. 209.

[2] P. Mazur and E. W. Montroll, J. Math. Phys. 1, 70 (1960).

[3] See A. W. Conway and A. J. McConnell, *The Mathematical Papers of Sir William Rowan Hamilton* (Cambridge University Press, New York, 1940), Vol. 2, pp. 451-582, 599.

[4] The one-dimensional lattice containing a heavy particle has been studied by two authors: (a) R. J. Rubin, *Proceedings of the International Symposium on Transport Processes in Statistical Mechanics, August 1956*, I. Prigogine, Editor (Interscience Publishers, Inc., New York, 1958), p. 155. In this paper a velocity autocorrelation function for the heavy particle is obtained. [Although Eq. (14) of the reference is in error, the final form of the autocorrelation function Eq. (19) is correct.] (b) P. C. Hemmer, footnote reference 6, obtains the conditional velocity distribution function in the one-dimensional case.

[5] S. Chandrasekhar, Revs. Modern Phys. 15, 1 (1943). See also footnote references 4a and 4b.

[6] P. C. Hemmer, Det Fysiske Seminar i Trondheim 2 (1959).

masses of the other particles are m. A second modification, which is introduced merely as a formal convenience to make the potential energy matrix positive definite, is that each particle is held to its lattice site by a harmonic force (strength $=k'$). Ultimately we shall be interested in the limit $k'\to 0$. The equations of motion of the system for particle displacements in a given lattice direction are independent of the displacements in other lattice directions.[1] The equations of motion for the x component are

$$[m+(M-m)\delta_{\mathbf{0},\mathbf{R}}]x_{tt}[\mathbf{R},t]$$
$$=-k'x[\mathbf{R},t]+\sum_{j=1}^{n}k_j\{x[\mathbf{R}+\mathbf{l}_j,t]-2x[\mathbf{R},t]+x[\mathbf{R}-\mathbf{l}_j,t]\},\quad(1)$$

where a subscript t denotes differentiation with respect to time and $x[\mathbf{R},t]$ is the displacement from equilibrium in the x direction of particle $\mathbf{R}$. The vector $\mathbf{l}_j$ is a unit vector in the lattice direction j. The various nearest neighbor force constants are denoted by k_j and the Kronecker delta

$$\delta_{\mathbf{0},\mathbf{R}}=\begin{cases}1 & \text{if } \mathbf{R}=\mathbf{0}\\ 0 & \text{if } \mathbf{R}\neq\mathbf{0}.\end{cases}$$

Equations (1) are solved by introducing a generating function. If we multiply the equation for $x_{tt}[\mathbf{R},t]$ by $(2N+1)^{-n/2}\exp[(2\pi i/2N+1)\mathbf{S}\cdot\mathbf{R}]$ and sum the resulting set of equations, we obtain

$$G_{tt}[\mathbf{S},t]+(2N+1)^{-n/2}Qx_{tt}[\mathbf{0},t]$$
$$=-\gamma'G[\mathbf{S},t]-2\sum_{j=1}^{n}\gamma_j\left\{1-\cos\frac{2\pi s_j}{2N+1}\right\}G[\mathbf{S},t],\quad(2)$$

where the vector $\mathbf{S}$ has integer components $s_1,\cdots,s_n$ and $-N\leqslant s_j\leqslant N$. The generating function $G[\mathbf{S},t]$ is, by definition

$$G[\mathbf{S},t]=(2N+1)^{-n/2}\sum_{\{\mathbf{R}\}}x[\mathbf{R},t]\exp\left[\frac{2\pi i}{2N+1}\mathbf{S}\cdot\mathbf{R}\right],\quad(3)$$

where the sum is over all vectors $\mathbf{R}$. The parameters Q, γ', and γ_j are, respectively, $(M-m)/m$, k'/m, and k_j/m. Equation (2) for the generating function can be solved by the method of Laplace transforms.

The Laplace transform of Eq. (2) is

$$-G_t[\mathbf{S},0]-pG[\mathbf{S},0]+p^2\Gamma[\mathbf{S},p]$$
$$-(2N+1)^{-n/2}Q\{x_t[\mathbf{0},0]+px[\mathbf{0},0]-p^2\xi[\mathbf{0},p]\}$$
$$=\left\{-\gamma'-2\sum_{j=1}^{n}\gamma_j\left(1-\cos\frac{2\pi s_j}{2N+1}\right)\right\}\Gamma[\mathbf{S},p],\quad(4)$$

where $\Gamma[\mathbf{S},p]$ is the Laplace transform of $G[\mathbf{S},t]$, $\Gamma[\mathbf{S},p]=\int_0^\infty G[\mathbf{S},t]e^{-pt}dt$, and $\xi[\mathbf{0},p]$ is the transform of $x[\mathbf{0},t]$. In fact, there is the general relation

$$\Gamma[\mathbf{S},p]=(2N+1)^{-n/2}\sum_{\{\mathbf{R}\}}\xi[\mathbf{R},p]\exp\left\{\frac{2\pi i}{2N+1}\mathbf{S}\cdot\mathbf{R}\right\}.\quad(5)$$

$G_t[\mathbf{S},0]$ and $G[\mathbf{S},0]$ contain all initial conditions. If we solve Eq. (4) for $\Gamma[\mathbf{S},p]$, we obtain

$$\Gamma[\mathbf{S},p]=\frac{G_t[\mathbf{S},0]+pG[\mathbf{S},0]+(2N+1)^{-n/2}Q\{x_t[\mathbf{0},0]+px[\mathbf{0},0]-p^2\xi[\mathbf{0},p]\}}{p^2+\gamma'+2\sum_{j=1}^{n}\gamma_j\left(1-\cos\frac{2\pi s_j}{2N+1}\right)}.\quad(6)$$

It follows from the orthonormality of the quantities, $(2N+1)^{-n/2}\exp\{(2\pi i/2N+1)\mathbf{S}\cdot\mathbf{R}\}$, that if both sides of Eq. (6) are multiplied by $(2N+1)^{-n/2}$ and summed over all values of $\{\mathbf{S}\}$ that

$$\xi[\mathbf{0},p]=\sum_{\{\mathbf{R}\}}{}'\{x_t[\mathbf{R},0]+px[\mathbf{R},0]\}\zeta[\mathbf{R},p]$$
$$+(Q+1)\{x_t[\mathbf{0},0]+px[\mathbf{0},0]\}\zeta[\mathbf{0},p]$$
$$-Qp^2\xi[\mathbf{0},p]\zeta[\mathbf{0},p],\quad(7)$$

where the prime on the summation sign indicates that the $\mathbf{R}=\mathbf{0}$ term is omitted, and where

$$\zeta[\mathbf{R},p]=(2N+1)^{-n/2}$$
$$\times\sum_{\{\mathbf{S}\}}\left[p^2+\gamma'+2\sum_{j=1}^{n}\gamma_j\left(1-\cos\frac{2\pi s_j}{2N+1}\right)\right]^{-1}$$
$$\times\exp\left\{\frac{2\pi i}{2N+1}\mathbf{S}\cdot\mathbf{R}\right\}.\quad(7a)$$

On solving Eq. (7) for $\xi[\mathbf{0},p]$, the expression is

$$\xi[\mathbf{0},p]=(Q+1)\{x_t[\mathbf{0},0]+px[\mathbf{0},0]\}$$
$$\times\zeta[\mathbf{0},p]\{1+Qp^2\zeta[\mathbf{0},p]\}^{-1}$$
$$+\sum_{\{\mathbf{R}\}}{}'\{x_t[\mathbf{R},0]+px[\mathbf{R},0]\}$$
$$\times\zeta[\mathbf{R},p]\{1+Qp^2\zeta[\mathbf{0},p]\}^{-1}.\quad(8)$$

Expressions for $x[\mathbf{0},t]$ and $x_t[\mathbf{0},t]$ can be obtained by inverting the Laplace transforms in Eq. (8). In the next section, we will be exclusively concerned with the expression for $x_t[\mathbf{0},t]$,

$$x_t[\mathbf{0},t]=x_t[\mathbf{0},0]X_t[\mathbf{0},t]+x[\mathbf{0},0]X_{tt}[\mathbf{0},t]$$
$$+\frac{1}{Q+1}\sum_{\{\mathbf{R}\}}{}'\{x_t[\mathbf{R},0]\mathbf{X}_t[\mathbf{R},t]$$
$$+x[\mathbf{R},0]X_{tt}[\mathbf{R},t]\},\quad(9)$$

where

$$X[\mathbf{R},t]=\frac{Q+1}{2\pi i}\int_L \frac{\zeta[\mathbf{R},p]e^{pt}dp}{1+Qp^2\zeta[\mathbf{0},p]}. \tag{10}$$

The path of integration in Eq. (10) is a line parallel to the imaginary p axis and to the right of all singularities of the integrand. Equation (9) is an expression for the velocity of particle $\mathbf{0}$ as a linear combination of initial positions and velocities.[7]

We will now show that the set of functions, $\{X[\mathbf{R},t]\}$, from which the time-dependent coefficients in Eq. (9) can be derived, is a solution of the equations of motion (1) for a particular initial condition. Consider the expression Eq. (6) for the generating function for the case in which the only nonzero initial value is $x_t[\mathbf{0},0]$, i.e.,

$$\begin{aligned} x[\mathbf{R},0]&=0, \quad \text{all } \mathbf{R} \\ x_t[\mathbf{R},0]&=\delta_{\mathbf{R},0}. \end{aligned} \tag{11a}$$

The Laplace transform of $G[\mathbf{S},t]$ is, in this case,

$$\Gamma[\mathbf{S},p]=\frac{(2N+1)^{-n/2}\{Q+1-Qp^2\xi[\mathbf{0},p]\}}{p^2+\gamma'+2\sum_{j=1}^{n}\gamma_j\left(1-\cos\frac{2\pi s_j}{2N+1}\right)}. \tag{11}$$

If Eq. (11) is multiplied by

$$(2N+1)^{-n/2}\exp\{-(2\pi i/2N+1)\mathbf{S}\cdot\mathbf{R}\},$$

$\mathbf{R}\neq\mathbf{0}$ and summed over all $\mathbf{S}$, one obtains an expression for $\xi[\mathbf{R},p]$, the transform of $x[\mathbf{R},t]$ [see Eq. (5)], in terms of the transform of $x[\mathbf{0},t]$,

$$\xi[\mathbf{R},p]=(Q+1)\zeta[-\mathbf{R},p]-Qp^2\xi[\mathbf{0},p]\zeta[-\mathbf{R},p]. \tag{12}$$

The expression for $\xi[\mathbf{0},p]$ for the initial condition (11a) is, according to Eq. (8),

$$\xi[\mathbf{0},p]=(Q+1)\zeta[\mathbf{0},p]/(1+Qp^2\zeta[\mathbf{0},p]). \tag{13}$$

On substituting this expression in Eq. (12), $\xi[\mathbf{R},p]$ can be rewritten as

$$\xi[\mathbf{R},p]=(Q+1)\zeta[-\mathbf{R},p]/(1+Qp^2\zeta[\mathbf{0},p]). \tag{14}$$

Upon inverting Eqs. (13) and (14), it is seen that

$$\begin{aligned} x[\mathbf{R},t]&=X[-\mathbf{R},t] \\ &=X[\mathbf{R},t], \end{aligned} \tag{15}$$

where $X[\mathbf{R},t]$ is defined in Eq. (10). It has thus been shown that the time-dependent contribution to $x_t[\mathbf{0},t]$ of arbitrary nonzero values of $x[\mathbf{R},0]$ and $x_t[R,0]$ in Eq. (9) can be expressed in terms of time derivatives of the function $X[\mathbf{R},t]$, where the functions $\{X[\mathbf{R},t]\}$ constitute a set of solutions of the equations of motion (1) for the initial conditions (11a).

In order to express concisely the relation which has been established between the time-dependent coefficients in Eq. (9) and the solution of the equations of motion, $\{X[\mathbf{R},t]\}$, and to simplify the rest of the analysis, we introduce a matrix notation. The equations of motion (1) in matrix form are

$$\mathbf{M}\mathbf{X}_{tt}(t)=\mathbf{V}\mathbf{X}(t), \tag{16}$$

where $\mathbf{M}$ is the diagonal mass matrix with elements

$$m\delta_{\mathbf{R},\mathbf{R}'}+(M-m)\delta_{\mathbf{0},\mathbf{R}'},$$

where $\mathbf{V}$ is the potential energy matrix for the system of particles [the matrix of the coefficients on the right-hand side of Eq. (1)], and where $\mathbf{X}(t)$, the particular solution chosen for illustration, is the vector whose components are $X[\mathbf{R},t]$. In terms of the foregoing quantities, the velocity of particle $\mathbf{0}$, Eq. (9), at time t, for arbitrary initial conditions, can be rewritten as

$$\begin{aligned} x_t[\mathbf{0},t]&=M^{-1}\{\mathbf{x}_t(0)^T\mathbf{M}\mathbf{X}_t(t)+\mathbf{x}(0)^T\mathbf{M}\mathbf{X}_{tt}(t)\} \\ &=M^{-1}\{\mathbf{x}_t(0)^T\mathbf{M}\mathbf{X}_t(t)+\mathbf{x}(0)^T\mathbf{V}\mathbf{X}(t)\}, \end{aligned} \tag{17}$$

where use is made of Eq. (16), where the initial conditions $x[\mathbf{R},0]$ and $x_t[\mathbf{R},0]$ are expressed as the vectors, $\mathbf{x}(0)$ and $\mathbf{x}_t(0)$, and where $\mathbf{x}(0)^T$ denotes the transpose of $\mathbf{x}(0)$.

III. VELOCITY DISTRIBUTION FUNCTION

One of the principal objectives of this work is to obtain a conditional velocity distribution function for the heavy particle $\mathbf{0}$. At the end of the preceding section, an explicit expression for the velocity of particle $\mathbf{0}$ at time t was obtained in the form of a linear combination of the initial conditions $\mathbf{x}_t(0)$ and $\mathbf{x}(0)$ for the system of $(2N+1)^n$ particles. In order to proceed, it will be assumed that the initial positions and velocities are canonically distributed, i.e., the distribution function for the initial x components of motion is

$$\begin{aligned} &\mathcal{W}[\mathbf{x}_t(0),\mathbf{x}(0)] \\ &\quad=\mathfrak{N}\exp\{-(1/2kT)[\mathbf{x}_t(0)^T\mathbf{M}\mathbf{x}_t(0)+\mathbf{x}(0)^T\mathbf{V}\mathbf{x}(0)]\}, \end{aligned} \tag{18}$$

where $\mathfrak{N}$ is a normalization constant. With this assumption, the expression for the conditional velocity distribution, $P(v,t|v_0,0)$, the probability that the velocity of particle $\mathbf{0}$ is v at time t when it was v_0 at time zero, is

$$P(v,t|v_0,0)=\frac{\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}_t(0)\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}(0)\delta\{v-M^{-1}[\mathbf{x}_t(0)^T\mathbf{M}\mathbf{X}_t(t)+\mathbf{x}(0)^T\mathbf{V}\mathbf{X}(t)]\}\delta\{x_t[\mathbf{0},0]-v_0\}\mathcal{W}[\mathbf{x}_t(0),\mathbf{x}(0)]}{\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}_t(0)\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}(0)\delta\{x_t[\mathbf{0},0]-v_0\}\mathcal{W}[\mathbf{x}_t(0),\mathbf{x}(0)]}, \tag{19}$$

[7] Similar types of results have been obtained for the uniform lattice by Hamilton[3] and more recently by R. E. Peierls, Proc. Natl. Inst. Sci. India **20**, 121 (1954).

where $\delta\{\ \}$ is a Dirac δ function. By using an integral representation for the δ functions in Eq. (19), the integrations can be performed (see Appendix A), and the following simple result is obtained:

$$P(v,t|v_0,0)=[2\pi kTM^{-1}\{1-X_t^2[\mathbf{0},t]\}]^{-\frac{1}{2}} \times\exp\left[-\frac{M\{v-v_0X_t[\mathbf{0},t]\}^2}{2kT\{1-X_t^2[\mathbf{0},t]\}}\right], \quad (20)$$

where $X_t[\mathbf{0},t]$ is the velocity of particle $\mathbf{0}$ at time t corresponding to the special initial conditions (11a). This result is a generalization of the results of Mazur and Montroll[2] and Hemmer.[6]

The conditional mean velocity, or autocorrelation function of the heavy particle, is

$$\langle v(t)\rangle=v_0X_t[\mathbf{0},t] \quad (21)$$

and the dispersion about the mean $\sigma^2(t)=\langle v^2(t)\rangle-\langle v(t)\rangle^2$ is

$$\sigma^2(t)=kTM^{-1}\{1-X_t^2[\mathbf{0},t]\}. \quad (22)$$

Thus the time-dependence of both parameters characterizing the distribution function $P(v,t|v_0,0)$ is determined solely by the autocorrelation function $X_t[\mathbf{0},t]$. It should be mentioned here that it can easily be shown that the distribution function for the velocity of particle $\mathbf{0}$, $w(x_t[\mathbf{0},0])$, which was assumed initially, is preserved in the course of time. That is, $w(x_t[\mathbf{0},0])$ defined by

$$w(x_t[\mathbf{0},0]) =\int_{-\infty}^{\infty}\cdots\int'd\mathbf{x}_t(0)\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}(0)\mathcal{W}[\mathbf{x}_t(0),\mathbf{x}(0)] =(2\pi kTM^{-1})^{-\frac{1}{2}}\exp\{-Mx_t^2[\mathbf{0},0]/2kT\},$$

where the prime indicates that the integration over $x_t[\mathbf{0},0]$ is omitted, has the same form as the velocity distribution for particle $\mathbf{0}$ at time t

$$P(v,t)=\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}_t(0)\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}(0) \times\delta\{v-M^{-1}[\mathbf{x}(0)^T\mathbf{M}\mathbf{X}_t(t)+\mathbf{x}(0)^T\mathbf{V}\mathbf{X}(t)]\} \times\mathcal{W}[\mathbf{x}_t(0),\mathbf{x}(0)] =(2\pi kTM^{-1})^{-\frac{1}{2}}\exp\{-Mv^2/2kT\}.$$

Obviously, this result is to be expected. Nevertheless, it is surprising that it can be obtained in such a trivial fashion.

IV. PROPERTIES OF THE VELOCITY AUTOCORRELATION FUNCTION $X_t[\mathbf{0},t]$

In this section we first discuss some general properties of the autocorrelation function $X_t[\mathbf{0},t]$ in the limits in which $\gamma'\to 0$ and $N\to\infty$; and then we obtain expressions for $X_t[\mathbf{0},t]$ in the case of the one- and two-dimensional lattices when $m/M\ll 1$ (the n-dimensional lattice will be referred to as an nD lattice). The passage to the limit $\gamma'=0$ is a trivial one. The parameter γ' was introduced to facilitate the integrations in Eq. (19). In the limit $N=\infty$, the summation in Eq. (7a) is replaced by an integration and the discrete variable $2\pi s_j/(2N+1)$ by the continuous variable θ_j. According to Eqs. (10) and (7a), in the limit $\gamma'=0$ and $N=\infty$,

$$X_t[\mathbf{0},t]=\frac{Q+1}{2\pi i}\int_L\frac{e^{pt}dp}{Qp+(p\zeta[\mathbf{0},p])^{-1}}, \quad (23)$$

where

$$\zeta[\mathbf{0},p]=\left(\frac{1}{2\pi}\right)^n\int_{-\pi}^{\pi}\cdots\int d\theta_1\cdots d\theta_n \times[p^2+2\sum_{j=1}^{n}\gamma_j(1-\cos\theta_j)]^{-1}. \quad (24)$$

The following alternative form of $\zeta[\mathbf{0},p]$ can be obtained from Eq. (24) by replacing

$$[p^2+2\sum_{j=1}^{n}\gamma_j(1-\cos\theta_j)]^{-1}$$

by

$$\int_0^{\infty}du\exp\{-u[p^2+2\sum_{j=1}^{n}\gamma_j(1-\cos\theta_j)]\}$$

and noting that the integral representation of the Bessel function $J_0(x)$ is $(2\pi)^{-1}\int_{-\pi}^{\pi}d\theta\exp(-ix\cos\theta)$,

$$\zeta[\mathbf{0},p]=\int_0^{\infty}du \times\exp(-p^2u)\prod_{j=1}^{n}\{\exp(-2\gamma_ju)J_0(2i\gamma_ju)\}. \quad (25)$$

In the $1D$ and $2D$ lattices, $\zeta[\mathbf{0},p]$ is, respectively,[8]

$$\zeta[\mathbf{0},p]=p^{-1}[p^2+4\gamma]^{-\frac{1}{2}} \quad (26)$$

and

$$\zeta[\mathbf{0},p]=(p^2+4\gamma_1)^{-\frac{1}{2}}(p^2+4\gamma_2)^{-\frac{1}{2}} \times{}_2F_1[\tfrac{1}{2},\tfrac{1}{2};1;16\gamma_1\gamma_2(p^2+4\gamma_1)^{-1}(p^2+4\gamma_2)^{-1}], \quad (27)$$

where ${}_2F_1[\ ]$ is a hypergeometric function.

As an indication of different dynamical behavior in the $1D$ and $2D$ lattices, consider the value of the following integral:

$$\Delta X=\int_0^{\infty}X_t[\mathbf{0},t]dt. \quad (28)$$

The distance ΔX is the net displacement of particle $\mathbf{0}$ in

[8] A. Erdelyi, W. Magnus, F. Oberhettinger, and F. Tricomi, *Tables of Integral Transforms* (McGraw-Hill Book Company, Inc., New York, 1954), Vol. 1. An expression for $\zeta[\mathbf{0},p]$ for the general nD lattice can also be found in this reference.

the case of the special initial conditions (11a), as well as the integral of the autocorrelation function. A general expression for ΔX is

$$\Delta X=\lim_{p\to 0}\frac{(Q+1)p\zeta[\mathbf{0},p]}{1+Qp^2\zeta[\mathbf{0},p]}; \tag{29}$$

and in the $1D$ and $2D$ lattices ΔX has the values $(Q+1)(4\gamma)^{-\frac{1}{2}}$ and 0, respectively. It can thus be seen that in the $1D$ lattice, particle $\mathbf{0}$ and its neighbors come to rest a distance ΔX from their initial positions whereas in the $2D$ lattice, particle $\mathbf{0}$ behaves as if it were moving in a potential well with a minimum at its initial position.[9] These different dynamical properties are undoubtedly related to the corresponding localizability properties of particles in such lattices discussed by Peierls,[10] Wigner,[11] and Montroll.[1]

We will now obtain expressions for $X_t[\mathbf{0},t]$ in the $1D$ and $2D$ lattices. The calculation of $X_t[\mathbf{0},t]$ for the $3D$ lattice will be reported in a later publication.

(a) $1D$ Lattice

In the case of the $1D$ lattice, the expression for $X_t[\mathbf{0},t]$, which is obtained by substituting Eq. (26) in Eq. (23), is

$$X_t[\mathbf{0},t]=\frac{Q+1}{2\pi i}\int_L\frac{\exp(2\gamma^{\frac{1}{2}}\rho t)d\rho}{Q\rho+(1+\rho^2)^{\frac{1}{2}}}, \tag{30}$$

where p has been replaced by $2\gamma^{\frac{1}{2}}\rho$. There are two values of Q for which the value of $X_t[\mathbf{0},t]$ is readily obtained, namely $Q=0$ and $Q=1$ ($M=m$ and $M=2m$, respectively),

$$X_t[\mathbf{0},t]=\begin{cases}J_0(\tau), & M=m,\\ 2\tau^{-1}J_1(\tau), & M=2m,\end{cases}$$

where $\tau=2\gamma^{\frac{1}{2}}t$, and where $J_0(\tau)$ and $J_1(\tau)$ are Bessel functions of the first kind. The former result for the uniform lattice is a relatively old one.[3,12] Since, in this work, we are interested in these lattices as models for the study of Brownian motion, we will confine our attention to the case in which $M\gg m(Q\gg 1)$.

The integrand in Eq. (30) has two branch points, at $\rho=i$ and $-i$. A cut can be drawn between the branch points as shown in Fig. 1; then the path of integration, L can be deformed into a closed contour C as shown. It can readily be verified that the integrand has a simple pole at $\rho_0=-(Q^2-1)^{-\frac{1}{2}}$ (and when $Q>1$, ρ_0 is real). The contour C can be deformed so that $X_t[\mathbf{0},t]$ in Eq. (30) can be expressed as the sum of two terms, the residue at

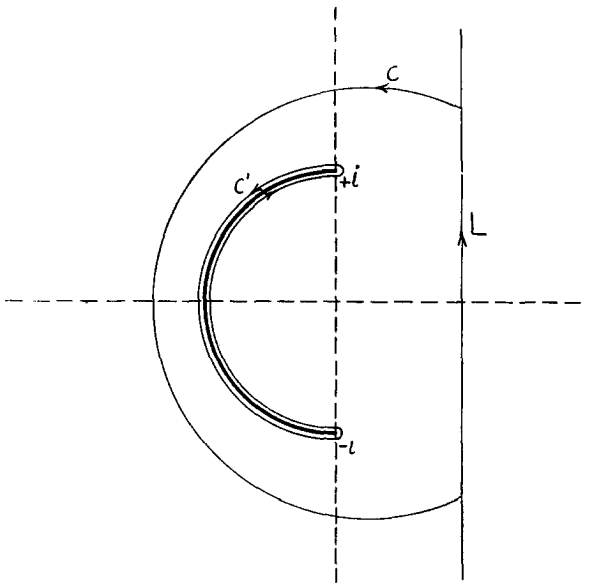

FIG. 1. The cut is a semicircular arc of unit radius in the ρ plane.

$\rho_0=-(Q^2-1)^{-\frac{1}{2}}$ and $\delta_1X_t(t)$, the value of the line integral around C',

$$X_t[\mathbf{0},t]=\frac{Q+1}{Q-Q^{-1}}\exp[-\tau(Q^2-1)^{-\frac{1}{2}}]+\frac{Q+1}{2\pi i}\int_{C'}\frac{e^{\rho\tau}d\rho}{Q\rho+(1+\rho^2)^{\frac{1}{2}}}. \tag{31}$$

It is shown in Appendix B that $|\delta_1X_t(t)|\leqslant 2^{\frac{1}{2}}Q^{-1}$, a bound which is independent of the time. Thus, in the limit $Q\gg 1$ and for times t which are not too large, the autocorrelation function $X_t[\mathbf{0},t]$ is

$$X_t[\mathbf{0},t]\cong e^{-\tau/Q}, \tag{32}$$

a result obtained by Hemmer,[6] and Rubin.[4a] The decay constant or relaxation time

$$\tau_R=Q/2\gamma^{\frac{1}{2}}$$

is such that in the time τ_R, a wave front originating at particle $\mathbf{0}$ and traveling with the velocity of very long waves in the lattice $\gamma^{\frac{1}{2}}$ will pass over a number of light particles whose total mass is M. Note further that the initial acceleration or initial slope of the autocorrelation curve plotted as a function of the time is not given accurately by Eq. (32). The exact value $X_{tt}[\mathbf{0},0]=0$ results from a cancellation of the derivative of the term shown in Eq. (32) with the derivative of the negligible correction term, since they are both of order $1/Q$. The form of Eq. (32) which is correct to the first order in $1/Q$ can be shown to be

$$X_t[\mathbf{0},t]\cong e^{-\tau/Q}+Q^{-1}\left\{\tau\left[1-\int_0^\tau\sigma^{-1}J_1(\sigma)d\sigma\right]-J_0(\tau)\right\}.$$

[9] Particle $\mathbf{0}$ in an nD lattice ($n\geqslant 3$) behaves in a similar manner.
[10] R. E. Peierls, Ann. Inst. Henri Poincaré **5**, 177 (1935).
[11] E. Wigner, *Lecture Notes on Solid State Physics* (Princeton University Press, Princeton, New Jersey, 1948).
[12] Sir W. R. Hamilton, Proc. Roy. Irish Acad. **1**, 267, 341 (1839); T. H. Havelock, Phil. Mag. **19**, 160 (1910); E. Schrödinger, Ann. Phys. **44**, 916 (1914).

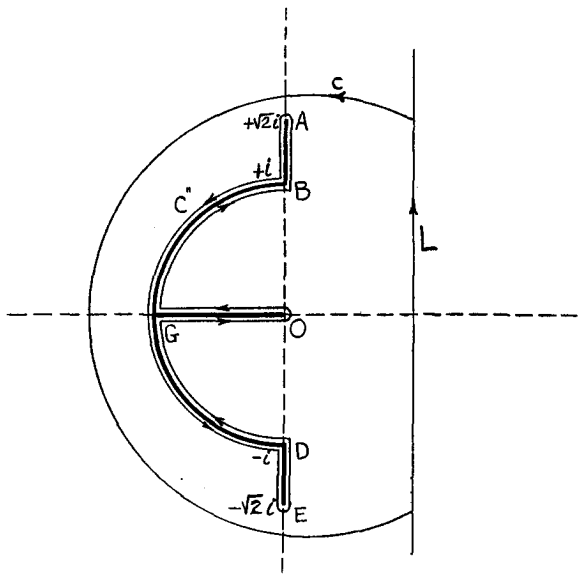

FIG. 2. The curved portion of the cut in the ρ plane is a semicircular arc of unit radius. The poles at $\rho_\pm$ are outside the contour C''.

(b) 2D Lattice

In the case of the $2D$ lattice, the expression for $X_\iota[\mathbf{0},t]$ is

$$X_\iota[\mathbf{0},t]=\frac{Q+1}{2\pi i}\times\int_L\frac{e^{\rho\tau}d\rho}{Q\rho+\rho^{-1}(\rho^2+1)/{}_2F_1[\frac{1}{2},\frac{1}{2};1;(\rho^2+1)^{-2}]},\tag{33}$$

where it has been assumed that $\gamma_1=\gamma_2=\gamma$ to simplify the discussion. The integrand in Eq. (33) has logarithmic singularities at $\rho=0$, $\pm i$, and $\pm 2^{\frac{1}{2}}i$. A cut can be drawn connecting these points, as shown in Fig. 2. As in the $1D$ case, the path of integration L can be deformed into a closed contour C as shown. It is shown in Appendix C that the integrand contains two poles, at $\rho_\pm=a\exp[\pm i(\frac{1}{2}\pi+\delta)]$ where $a\ll 1$; and that as $Q\to\infty$, a and δ are determined by the relations

$$\begin{aligned}&Q\cong\pi/a^2\ln(8/a^2)\\ \text{and}\qquad&\\ &\delta\cong\pi/2\ln(8/a^2).\end{aligned}\tag{34}$$

Proceeding as in the $1D$ case, the path of integration C can be deformed into C'' (see Fig. 2); and $X_\iota[\mathbf{0},t]$ can be expressed as a sum of terms, the sum of the residues at the two poles, $\rho_\pm=a\exp[\pm i(\frac{1}{2}\pi+\delta)]$ and the line integral around C'',

$$\begin{aligned}X_\iota[\mathbf{0},t]&=\mathrm{Res}(t)+\delta_2X_\iota(t)\\&=\frac{e^{-a\tau\sin\delta}}{1+\dfrac{1-2\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}}\\&\quad\times\left\{\left[1-\frac{\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}\right]\cos(a\tau\cos\delta)\right.\\&\quad\left.-\left[\frac{\pi+2\delta}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}\right]\sin(a\tau\cos\delta)\right\}\\&\quad+\delta_2X_\iota(t).\end{aligned}\tag{35}$$

Details are given in Appendix C. For the range of Q of interest, $\delta_2X_\iota(t)$ contributes a relatively small, though not negligible, negative correction to the right-hand side of Eq. (35). In Table I, some pertinent values of the parameters are given. The column labeled Res(0) is the value of Res (t) at $t=0$. As can be seen, Res(0) overestimates the value of $X_\iota[\mathbf{0},0]$, which is unity. The last column is an approximate value of Res(0) obtained by an expansion of Eq. (C17) in powers of $[\ln(8/a^2)]^{-1}$. As shown in Appendix C, the correction $\delta_2X_\iota(t)$ decreases in magnitude but is always negative.

An approximate form for the autocorrelation function $X_\iota[\mathbf{0},t]$ when $[\ln(8/a^2)]^{-1}\ll 1$ is

$$X_\iota[\mathbf{0},t]\cong\cos(a\tau)\exp[-\pi a\tau/2\ln(8/a^2)].\tag{36}$$

The decay constant in the exponential is relatively large compared to the period of the cosine factor. For the set of parameters in Table I associated with $Q=40\,800$, the value of $X_\iota[\mathbf{0},t]$ when $\cos\alpha\tau=-1$ is $X_\iota[\mathbf{0},t]=-0.73$. As an indication that the correction $\delta_2X_\iota(t)$ is significant in the limit of large Q, the integral of $X_\iota[\mathbf{0},t]$ in Eq. (35) with respect to the time is

$$\Delta X\cong\delta/a.$$

This value should be compared with the exact result, zero, obtained from Eq. (29).

TABLE I.

Q	a	$\pm\delta$	$\ln(a^2/8)$	Res(0)	$1+[\ln(8/a^2)]^{-1}$
127	$10^{-1.5}$	±0.1863	-8.99	1.105	1.111
811	$10^{-2.0}$	±0.1483	-11.29	1.087	1.089
5590	$10^{-2.5}$	±0.1232	-13.59	1.074	1.074
40 800	$10^{-3.0}$	±0.1053	-15.89	1.063	1.063

ACKNOWLEDGMENT

I wish to thank Dr. R. W. Zwanzig for several helpful discussions.

APPENDIX A. VELOCITY DISTRIBUTION FUNCTION

On replacing the δ functions in Eq. (19) by their integral representations, the expression for $P(v,t|v_0,0)$

can be written as

$$P(v,t|v_0,0)=\frac{\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}_t(0)\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}(0)\int_{-\infty}^{\infty}\frac{ds}{2\pi}\int_{-\infty}^{\infty}\frac{dr}{2\pi}\exp\left\{is[v-M^{-1}\mathbf{x}_t(0)^T\mathbf{M}\mathbf{X}_t(t)-M^{-1}\mathbf{x}(0)^T\mathbf{V}\mathbf{X}(t)]\right.}{\left.+ir[v_0-\mathbf{x}_t(0)^T\boldsymbol{\Delta}]-\frac{1}{2kT}[\mathbf{x}_t(0)^T\mathbf{M}\mathbf{x}_t(0)+\mathbf{x}(0)^T\mathbf{V}\mathbf{x}(0)]\right\}}$$
$$\frac{\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}_t(0)\int_{-\infty}^{\infty}\cdots\int d\mathbf{x}(0)\int_{-\infty}^{\infty}\frac{dr}{2\pi}\exp\left\{ir[v_0-\mathbf{x}_t(0)^T\boldsymbol{\Delta}]\right.}{\left.-\frac{1}{2kT}[\mathbf{x}_t(0)^T\mathbf{M}\mathbf{x}_t(0)+\mathbf{x}(0)^T\mathbf{V}\mathbf{x}(0)]\right\}}, \tag{A1}$$

where, for convenience, the scalar $x_t[\mathbf{0},0]$ has been replaced by the scalar product $\mathbf{x}_t(0)^T\cdot\boldsymbol{\Delta}$. All components of $\boldsymbol{\Delta}$ are zero, except the $\mathbf{0}$ component which is equal to unity. The integrations over $\mathbf{x}_t(0)$ and $\mathbf{x}(0)$ in Eq. (19) can be performed by using the following general relation[13]:

$$\int_{-\infty}^{\infty}\cdots\int d\mathbf{z}\,\exp\{i\mathbf{t}^T\mathbf{z}-\tfrac{1}{2}\mathbf{z}^T\mathbf{A}\mathbf{z}\}=\frac{(2\pi)^{n/2}}{(|A|)^{\frac{1}{2}}}\exp\{-\tfrac{1}{2}\mathbf{t}^T\mathbf{A}^{-1}\mathbf{t}\}, \tag{A2}$$

where $\mathbf{A}$ is a positive definite matrix of order n, $|A|$ denotes the determinant of $\mathbf{A}$, and $\mathbf{A}^{-1}$ the inverse of $\mathbf{A}$. The result is

$$P(v,t|v_0,0)=\frac{\int_{-\infty}^{\infty}\frac{ds}{2\pi}\int_{-\infty}^{\infty}\frac{dr}{2\pi}\exp\left\{isv+irv_0-\frac{kT}{2}[sM^{-1}\mathbf{M}\mathbf{X}_t(t)+r\boldsymbol{\Delta}]^T\mathbf{M}^{-1}[sM^{-1}\mathbf{M}\mathbf{X}_t(t)+r\boldsymbol{\Delta}]\right.}{\left.-\frac{kT}{2}s^2M^{-2}[\mathbf{V}\mathbf{X}(t)]^T\mathbf{V}^{-1}[\mathbf{V}\mathbf{X}(t)]\right\}}$$
$$\int_{-\infty}^{\infty}\frac{dr}{2\pi}\exp\left\{irv_0-\frac{kT}{2}r^2\boldsymbol{\Delta}\mathbf{M}^{-1}\boldsymbol{\Delta}\right\} \tag{A3}$$

$$=\frac{\int_{-\infty}^{\infty}\frac{ds}{2\pi}\exp\left\{isv-\frac{kT}{2}s^2M^{-2}[\mathbf{X}_t(t)^T\mathbf{M}\mathbf{X}_t(t)+\mathbf{X}(t)^T\mathbf{V}\mathbf{X}(t)]\right.}{\left.-[v_0+ikTsM^{-1}\boldsymbol{\Delta}^T\mathbf{X}_t(t)]^2/[2kT\boldsymbol{\Delta}^T\mathbf{M}^{-1}\boldsymbol{\Delta}]\right\}}{\exp\{-v_0^2/[2kT\boldsymbol{\Delta}^T\mathbf{M}^{-1}\boldsymbol{\Delta}]\}}, \tag{A4}$$

where the existence of $\mathbf{V}^{-1}$ in Eq. (A3) has been insured by the addition of the weak force constants k'. The following relations are used to simplify Eq. (A4):

$$\boldsymbol{\Delta}^T\mathbf{M}^{-1}\boldsymbol{\Delta}=M^{-1}$$
$$\boldsymbol{\Delta}^T\mathbf{X}_t(t)=X_t[\mathbf{0},t]$$

and

$$\tfrac{1}{2}[\mathbf{X}_t(t)^T\mathbf{M}\mathbf{X}_t(t)+\mathbf{X}(t)^T\mathbf{V}\mathbf{X}(t)]=M/2.$$

The last relation is an expression for the total lattice energy corresponding to the initial conditions (11a). The final expression for $P(v,t|v_0,0)$ is

$$P(v,t|v_0,0)=\int_{-\infty}^{\infty}\frac{ds}{2\pi}\exp\left\{is(v-v_0X_t[\mathbf{0},t])-\frac{kT}{2}s^2M^{-1}(1-X_t^2[\mathbf{0},t])\right\}$$
$$=[2\pi kTM^{-1}(1-X_t^2[\mathbf{0},t])]^{-\frac{1}{2}}\exp\left[-\frac{M\{v-v_0X_t[\mathbf{0},t]\}^2}{2kT(1-X_t^2[\mathbf{0},t])}\right]. \tag{A5}$$

[13] H. Cramér, *Mathematical Methods of Statistics* (Princeton University Press, Princeton, New Jersey, 1946), p. 119.

APPENDIX B. UPPER BOUND OF THE CONTOUR INTEGRAL AROUND C', $\delta_1 X_t(t)$

The contour integral around C' in Fig. 1 is equal to the difference of two integrals along the semicircular cut

$$\delta_1 X_t(t)=\frac{Q+1}{2\pi}\int_{3\pi/2}^{\pi/2} d\theta\,\exp\{i\theta+\tau e^{i\theta}\}\left[\frac{1}{Qe^{i\theta}+(1+e^{2i\theta})^{\frac{1}{2}}}-\frac{1}{Qe^{i\theta}-(1+e^{2i\theta})^{\frac{1}{2}}}\right]$$

$$=\frac{Q+1}{\pi}\int_{/2}^{3\pi/2} d\theta\,\exp\{i\theta+\tau e^{i\theta}\}\frac{(1+e^{2i\theta})^{\frac{1}{2}}}{(Q^2-1)e^{2i\theta}-1}. \tag{B1}$$

An upper bound on the integral (B1) is

$$|\delta_1 X_t(t)|\leqslant\frac{Q+1}{\pi}\int_{\pi/2}^{3\pi/2} d\theta\,\exp\{\tau\cos\theta\}\frac{|(1+e^{2i\theta})^{\frac{1}{2}}|_{\max}}{|(Q^2-1)e^{2i\theta}-1|_{\min}}, \tag{B2}$$

where the pairs of vertical bars with the subscripts max and min denote, respectively, the maximum and minimum absolute magnitude. On inserting the values of the maximum and minimum magnitudes in Eq. (B2), and noting that the maximum value of $\exp(\tau\cos\theta)$ is unity in the interval of integration, an upper bound of $|\delta_1 X_t(t)|$ is

$$|\delta_1 X_t(t)|\leqslant\frac{Q+1}{\pi}\int_{\pi/2}^{3\pi/2} d\theta\frac{2^{\frac{1}{2}}}{Q^2-2}$$

$$\leqslant 2^{\frac{1}{2}}Q^{-1},\quad \text{for } Q\gg 1.$$

APPENDIX C. SOME DETAILS OF THE EVALUATION OF THE AUTOCORRELATION FUNCTION IN THE 2D LATTICE

1. Roots of $Q\varrho+\varrho^{-1}(\varrho^2+1)/{}_2F_1[\frac{1}{2},\frac{1}{2};1;(\varrho^2+1)^{-2}]=0$ for $Q\gg 1$ (C1)

In the neighborhood of $\rho=0$, the hypergeometric function ${}_2F_1[\frac{1}{2},\frac{1}{2};1;(\rho^2+1)^{-2}]$ can be written as[14]

$${}_2F_1[\tfrac{1}{2},\tfrac{1}{2};1;(\rho^2+1)^{-2}]$$

$$=-\frac{1}{\pi}\ln\frac{(\rho^2+1)^2}{\rho^2(\rho^2+2)}\,{}_2F_1\left[\tfrac{1}{2},\tfrac{1}{2};1;\frac{\rho^2(\rho^2+2)}{(\rho^2+1)^2}\right]$$

$$+\frac{2}{\pi}\sum_{n=0}^{\infty}\{\psi(n+1)-\psi(n+\tfrac{1}{2})\}\frac{(\tfrac{1}{2})_n(\tfrac{1}{2})_n}{(1)_n(1)_n}\left[\frac{\rho^2(\rho^2+2)}{(\rho^2+1)^2}\right]^n$$

$$\cong-\frac{1}{\pi}\ln(\tfrac{1}{2}\rho^2)+\frac{2}{\pi}\{\psi(1)-\psi(\tfrac{1}{2})\}+\cdots,\quad |\rho|\ll 1, \tag{C2}$$

where $\psi(z)$ denoted the function $\psi(z)=d\ln\Gamma(z)/dz$. On using the relation[15]

$$\psi(1)-\psi(\tfrac{1}{2})=2\ln 2,$$

the approximate expression for ${}_2F_1[\frac{1}{2},\frac{1}{2};1;(\rho^2+1)^{-2}]$ for $|\rho|\ll 1$ is

$${}_2F_1[\tfrac{1}{2},\tfrac{1}{2};1;(\rho^2+1)^{-2}]\cong\pi^{-1}\ln(8/\rho^2). \tag{C3}$$

It can readily be verified that for $Q\gg 1$, the only possible roots of Eq. (C1) are located near $\rho=0$, where Eq. (C1) can be replaced by the simpler equation

$$Q\rho^2+\pi[\ln(8/\rho^2)]^{-1}=0. \tag{C4}$$

On replacing ρ by $a\exp[i(\frac{1}{2}\pi+\delta)]$, the pair of equations for the real and imaginary parts of Eq. (C4) is

$$Qa^2\cos(\pi+2\delta)=\frac{-\pi\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2} \tag{C5}$$

$$Qa^2\sin(\pi+2\delta)=\frac{\pi(\pi+2\delta)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}. \tag{C6}$$

Some solutions of Eqs. (C5) and (C6) are listed in Table I. This table was constructed with the aid of the relation,

$$\tan 2\delta/(\pi+2\delta)=[\ln(8/a^2)]^{-1}, \tag{C7}$$

obtained by dividing Eq. (C6) by (C5). Starting with a value of a, δ was determined from Eq. (C7); and then the associated value of Q was determined from Eq. (C5). For a given value of a, there are two values of $(\pi/2)+\delta$ which only differ in sign. In the limit of very large Q ($a\ll 1$), where $\ln(8/a^2)\gg 1$, an approximate set of equations can be obtained from (C7) and (C5), namely,

$$Qa^2\cong\pi[\ln(8/a^2)]^{-1} \tag{C8}$$

$$\delta\cong\tfrac{1}{2}\pi[\ln(8/a^2)]^{-1}. \tag{C9}$$

2. Sum of the Residues of the Integrand in Eq. (33)

The sum of the residues of the integrand in Eq. (33) is calculated in a straightforward manner using the

[14] A. Erdelyi, W. Magnus, F. Oberhettinger, and F. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, p. 110.

[15] W. Magnus and F. Oberhettinger, *Special Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1949), p. 3.

relation[16]

$$\mathrm{Res}\left(\frac{F(z)}{G(z)}\right)=\frac{1}{2\pi i}\oint\frac{F(z)}{G(z)}dz$$
$$=\sum_i\frac{F(z_i)}{G'(z_i)},$$

where $F(z)$ and $G(z)$ are analytic inside the contour of integration, but $G(z)$ has simple zeros at the points, z_i. As shown in the foregoing, the denominator in the integrand of Eq. (33) has simple zeros at $\rho_\pm=a\exp[\pm i(\pi/2+\delta)]$. Near $\rho=0$, the denominator $D(\rho)$ can be approximated by the expression

$$D(\rho)=Q\rho+\pi[\rho\ln(8/\rho^2)]^{-1}$$

and

$$D'(\rho_\pm)=2Q\{1-[\ln(8/\rho_\pm^2)]^{-1}\}.$$

After some tedious algebra, the expression for the sum of the residues of the integrand in Eq. (33) reduces to

$$\mathrm{Res}\left(\frac{(Q+1)\exp(\rho\tau)}{Q\rho+\rho^{-1}(\rho^2+1)/{}_2F_1[\ ]}\right)\cong\frac{\exp(-a\tau\sin\delta)}{1+\dfrac{1-2\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}}$$
$$\times\left\{\left[1-\frac{\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}\right]\cos(a\tau\cos\delta)-\left[\frac{\pi+2\delta}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}\right]\sin(a\tau\cos\delta)\right\}. \quad \text{(C10)}$$

3. Contour Integral around C'', $\delta_2X_t(t)$

The contour integral around C'' in Fig. 2 can be expressed as the sum of two parts: (1) the difference of line integrals on either side of the cut $ABGDE$, and (2) the difference of line integrals on either side of the portion of the cut OG,

$$\delta_2X_t(t)=\frac{Q+1}{2\pi i}\int_{E\to A}d\rho e^{\rho\tau}\left\{\frac{1}{Q\rho+(\rho\zeta_R[\mathbf{0},\rho])^{-1}}-\frac{1}{Q\rho+(\rho\zeta_L[\mathbf{0},\rho])^{-1}}\right\}$$
$$+\frac{Q+1}{2\pi i}\int_{G\to0}d\rho e^{\rho\tau}\left\{\frac{1}{Q\rho+(\rho\zeta_D[\mathbf{0},\rho])^{-1}}-\frac{1}{Q\rho+(\rho\zeta_U[\mathbf{0},\rho])^{-1}}\right\}, \quad \text{(C11)}$$

where $\int_{E\to A}d\rho$ denotes the line integral from E to A along the cut $EDGBA$ and $\zeta_R[\mathbf{0},\rho]$ and $\zeta_L[\mathbf{0},\rho]$ denote, respectively, the values of $\zeta[\mathbf{0},\rho]$ on the right and left sides of the cut $EDGBA$. Similarly, $\int_{G\to0}d\rho$ denotes the line integral from G to 0 along the cut $G0$, and $\zeta_D[\mathbf{0},\rho]$ and $\zeta_U[\mathbf{0},\rho]$ denote, respectively, the values of $\zeta[\mathbf{0},\rho]$ on the lower and upper sides of the cut $G0$. By arguments similar to those used in Appendix B for the $1D$ case, the contribution of the first line integral in Eq. (C11) can be shown to be bounded by a quantity of order $1/Q$. Upon omitting this term and using Eq. (C2) for the analytic continuation of $\zeta_D[\mathbf{0},\rho]$ and $\zeta_U[\mathbf{0},\rho]$, the second line integral can be rewritten as

$$\delta_2X_t(t)=\frac{Q+1}{2\pi i}\int_{-1}^{0}dxe^{x\tau}\left\{\frac{x\zeta[\mathbf{0},xe^{-i\pi}]-x\zeta[\mathbf{0},xe^{i\pi}]}{(1+Qx^2\zeta[\mathbf{0},xe^{i\pi}])(1+Qx^2\zeta[\mathbf{0},xe^{-i\pi}])}\right\}. \quad \text{(C12)}$$

The explicit form of $\zeta[\mathbf{0},xe^{\pm i\pi}]$ is

$$\zeta[\mathbf{0},xe^{\pm i\pi}]=R(x)\pm iI(x), \quad \text{(C13)}$$

where

$$R(x)=\pi^{-1}(x^2+1)^{-1}\ln\frac{(x^2+1)^2}{x^2(x^2+2)}\,{}_2F_1\left[\tfrac{1}{2},\tfrac{1}{2};1;\frac{x^2(x^2+2)}{(x^2+1)^2}\right]$$
$$+2\pi^{-1}(x^2+1)^{-1}\sum_{n=0}^{\infty}\{\psi(n+1)-\psi(n+\tfrac{1}{2})\}\frac{(\frac{1}{2})_n(\frac{1}{2})_n}{(1)_n(1)_n}\left[\frac{x^2(x^2+2)}{(x^2+1)^2}\right]^n \quad \text{(C14)}$$

and

$$I(x)=-2(x^2+1)^{-1}\,{}_2F_1\left[\tfrac{1}{2},\tfrac{1}{2};1;\frac{x^2(x^2+2)}{(x^2+1)^2}\right]. \quad \text{(C15)}$$

[16] L. A. Pipes, *Applied Mathematics for Engineers and Physicists* (McGraw-Hill Book Company, Inc., New York, 1946), p. 464.

On using the quantities $R(x)$ and $I(x)$, and replacing x by $-y$, the final form for $\delta_2 X_t(t)$ is

$$\delta_2 X_t(t) \cong -\frac{2Q}{\pi}\int_0^1 dy e^{-\tau y}\frac{y(y^2+1)^{-1}\,{}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{y^2(y^2+2)}{(y^2+1)^2}\right]}{[1+Qy^2R(y)]^2+Q^2y^4I^2(y)}. \tag{C16}$$

Since the integrand in Eq. (C16) is positive, $\delta_2 X_t(t)$ constitutes a negative correction to the contribution of the residues to the autocorrelation function. The function $\delta_2 X_t(t)$ decreases with the time because of the presence of the factor, $\exp[-\tau y]$. The value of $\delta_2 X_t(t)$ at $t=0$ can be determined indirectly from the relation

$$X_t[0,0]=1$$
$$=\mathrm{Res}(t=0)+\delta_2 X_t(0).$$

With $\mathrm{Res}(t=0)$ determined from Eq. (C10), the value of $\delta_2 X_t(0)$ is

$$\delta_2 X_t(0)=1-\left\{1+\frac{1-2\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}\right\}^{-1}$$
$$\times\left\{1-\frac{\ln(8/a^2)}{[\ln(8/a^2)]^2+(\pi+2\delta)^2}\right\}. \tag{C17}$$

In the limit of very large Q, $\ln(8/a^2)$ is large compared to π (see Table I for typical values) and a simple approximate expression for $|\delta_2 X_t(0)|$, the maximum value of the magnitude of the negative quantity $\delta_2 X_t(t)$, is

$$|\delta_2 X_t(0)| \cong [\ln(8/a^2)]^{-1}. \tag{C18}$$

Analytic Properties of Radial Wave Functions*

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This is a review article about the properties of radial wave functions and other quantities relevant to the partial wave analysis of scattering theory, as functions of the energy or wave number. The treatment is restricted to the nonrelativistic Schrödinger equation for two particles with a local potential. In addition to regular and irregular solutions of the radial differential equations, the Jost function, S matrix, and Green's functions are analyzed and completeness is proved. The examples investigated in detail include the Bargmann potentials and their generalizations.

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1. INTRODUCTION

QUANTUM mechanics has undoubtedly its most beautiful general form in the language of abstract vector space theory, whose mathematical methods furnish it at the same time with one of its most powerful tools. There are nevertheless many fundamental problems which are attacked with advantage in a special representation. It has become clear lately that in nonrelativistic quantum mechanics as well as in relativistic field theory much can be gained by returning from the formal operator calculus to that of point functions. The theory of functions of complex variables, specifically, has become again a prominent tool of physics.

The recent upsurge of dispersion relation research is a case in point. Although its results can frequently be obtained without ever going into the complex plane, the most appropriate general mathematical tool is the theory of analytic functions.

Most physicists are quite conversant with the theory of differential and integral equations; most know also the essentials in the theory of functions. The combination of these two disciplines, however, is much less familiar to many. A useful purpose may therefore be served by reviewing what is known by means of complex analysis in a certain area of scattering theory.

I shall restrict myself to the nonrelativistic quantum mechanics of two-particle systems, that is, the one-particle Schrödinger equation in the center of mass system. The properties of the solutions of such a partial differential equation not being nearly as well understood as those of solutions of ordinary differential equations, a partial wave analysis is made which leads to single or coupled radial equations. The regular and irregular solutions of these as well as all the functions constructed from them for the purpose of scattering theory are to be investigated.

I shall restrict myself to local potentials. Certain types of nonlocality, such as spin-orbit forces introduce no changes whatever. Others may introduce only inessential complications. In the latter case references to appropriate papers will be given. The general case of nonlocal forces, however, is far more difficult and little is known about it.

The purpose of this article is not only to collect results; it is also didactic. The proofs therefore form an essential part of its methodological aim. How many physicists have actually seen a completeness proof, except for some very special functions?

Very little in this paper is new. Almost everything in it can be found in the published literature, directly or by implication. In contrast to some authors on the subject I shall not make a weak assumption concerning the potential and then stick to it. From time to time the assumptions will be explicitly strengthened in order to see what can be said then. The weakest hypothesis, always to be kept, is that the first and second absolute moments of the potential are finite; stronger ones to be made at various points are that the potential has an exponential tail or that it vanishes identically beyond a certain point. Since the earlier papers by Jost, Levinson, and others had a special purpose their authors were not interested in doing that explicitly, although some of the general consequences of a finite range follow immediately from their work and were known to them. How much more can be said if the potential vanishes beyond a point has been demonstrated particularly by the work of Humblet and Regge.

2. PRELIMINARIES ON SCATTERING THEORY

We start from the Schrödinger equation for two particles in the center of mass coordinate system:

$$[-(\hbar^2/2\mu)\nabla^2+H_I(\mathbf{r})]\psi(\mathbf{r})=E\psi(\mathbf{r}), \qquad (2.1)$$

μ being the reduced mass of the particles and $\mathbf{r}$, their

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relative distance. The interaction energy $H_I(\mathbf{r})$ is assumed to be invariant under rotations but may be spin dependent.

For the purpose of scattering theory it is advantageous to convert (2.1) into an integral equation which incorporates the boundary condition that at large distances the wave function should consist of a plane wave plus an outgoing spherical wave; thus, with $E=\hbar^2k^2/2\mu$,

$$\psi_+(\mathbf{k}s\nu,\mathbf{r})=\psi_0(\mathbf{k}s\nu,\mathbf{r}) + \int (d\mathbf{r})G_+(\mathbf{k};\mathbf{r},\mathbf{r}')H_I(\mathbf{r}')\psi_+(\mathbf{k}s\nu,\mathbf{r}), \quad (2.2)$$

where

$$\psi_0(\mathbf{k}s\nu,\mathbf{r})=[(\mu k)^{\frac{1}{2}}/\hbar(2\pi)^{\frac{3}{2}}]\chi_s{}^\nu e^{i\mathbf{k}\cdot\mathbf{r}},$$

χ being the relevant normalized spin wave function for the intrinsic angular momentum of the two particles. The normalization of ψ_0 is such that

$$\int (d\mathbf{r})\psi_0{}^*(\mathbf{k}s\nu,\mathbf{r})\psi_0(\mathbf{k}'s'\nu',\mathbf{r})=\delta(E-E')\delta(\Omega_k-\Omega_k')\delta_{ss'}\delta_{\nu\nu'},$$

$$\sum_{s\nu}\int_0^\infty dE\int d\Omega_k\psi_0{}^*(\mathbf{k}s\nu,\mathbf{r})\psi_0(\mathbf{k}s\nu,\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}');$$

Ω_k is the solid angle defined by $\mathbf{k}$.

The specification of *outgoing* spherical waves is accomplished by the choice of Green's function:

$$G_+(k;\mathbf{r},\mathbf{r}')=\sum_{s\nu}\int d\Omega_k'\int_0^\infty dE\frac{\psi_0{}^*(\mathbf{k}'s\nu,\mathbf{r})\psi_0(\mathbf{k}'s\nu,\mathbf{r}')}{E-E'+i\epsilon}$$

$$=-\frac{\mu}{2\pi\hbar^2}\frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}$$

$$\underset{r\to\infty}{\sim}-\frac{e^{ikr}}{r}\left(\frac{2\pi\mu}{k\hbar^2}\right)^{\frac{1}{2}}\sum_{s\nu}\chi_s{}^\nu\psi_0{}^*(\mathbf{k}''s\nu,\mathbf{r}'), \quad (2.3)$$

where $\mathbf{k}''\equiv k\mathbf{r}r^{-1}$.

We expand the Green's function and wave functions in spherical harmonics:

$$G_+(k;\mathbf{r},\mathbf{r}')=(2\mu/\hbar^2)\sum_{JMls}\mathcal{Y}_{Jls}{}^M(\mathbf{r})\mathcal{Y}_{Jls}{}^{M*}(\mathbf{r}') \times r^{-1}r'^{-1}G_l(k;r,r'), \quad (2.4)$$

$$G_l(k;r,r')=(-)^{l+1}k^{-1}u_l(kr_<)w_l(kr_>),$$

$$\psi_0(\mathbf{k}s\nu,\mathbf{r})=(2\mu k/\pi\hbar^2)^{\frac{1}{2}}(kr)^{-1}\sum_{JMlm}i^lu_l(kr) \times\mathcal{Y}_{Jls}{}^M(\mathbf{r})Y_l{}^{m*}(\mathbf{k})C_{ls}(J,M;m,\nu) \quad (2.5)$$

$$\psi(\mathbf{k}s\nu,\mathbf{r})=(2\mu k/\pi\hbar^2)^{\frac{1}{2}}(kr)^{-1}\sum_{JMll'ms'}i^l\psi_{l's',ls}{}^J(k,r) \times\mathcal{Y}_{Jl's'}{}^M(\mathbf{r})Y_l{}^{m*}(\mathbf{k})C_{ls}(J,M;m,\nu), \quad (2.6)$$

where $C_{ls}(J,M;m,\nu)$ are the Clebsch-Gordan coefficients in the notation of Blatt and Weisskopf,[1] and

$$\mathcal{Y}_{Jls}{}^M(\mathbf{r})=\sum_{m\nu}C_{ls}(J,M;m,\nu)Y_l{}^m(\mathbf{r})\chi_s{}^\nu.$$

Furthermore, we have used the Riccatti-Bessel functions

$$\begin{aligned}u_l(z)&\equiv zj_l(z)=(\tfrac{1}{2}\pi z)^{\frac{1}{2}}J_{l+\frac{1}{2}}(z)=(-)^{l+1}u_l(-z)\\ v_l(z)&\equiv zn_l(z)=(\tfrac{1}{2}\pi z)^{\frac{1}{2}}N_{l+\frac{1}{2}}(z)=(-)^lv_l(-z)\\ w_l(z)&\equiv -v_l(z)-iu_l(z)=-izh_l{}^{(2)}(z)\\ &=-i(\tfrac{1}{2}\pi z)^{\frac{1}{2}}H_{l+\frac{1}{2}}{}^{(2)}(z)=(-)^lw_l(-z)^*,\end{aligned} \quad (2.7)$$

which are most convenient for solving the radial equation. Insertion in (2.2) leads to a set of coupled integral equations for the radial functions:

$$\psi_{l's',ls}{}^J(k,r)=u_l(kr)\delta_{ll'}\delta_{ss'}+\sum_{l''s''}\int_0^\infty dr'G_{l'}(k;r,r') \times V_{l's',l''s''}{}^J(r')\psi_{l''s'',ls}{}^J(k,r'), \quad (2.8)$$

where

$$V_{ls,l's'}{}^J(r)=\frac{2\mu}{\hbar^2}\int d\Omega\mathcal{Y}_{Jls}{}^{M*}(\mathbf{r})H_I(\mathbf{r})\mathcal{Y}_{Jl's'}{}^M(\mathbf{r}). \quad (2.9)$$

The meaning of the subscripts on ψ follows from (2.6) and (2.8). The first set "$l's'$" indicates the component of ψ belonging to specific orbital and spin angular momenta, while the second set, "ls" refers to the angular momenta of the incident beam, i.e., to the boundary condition.

The solution of (2.8) satisfies the set of differential equations

$$-\frac{d^2}{dr^2}\psi_{l's',ls}{}^J+\sum_{l''s''}V_{l's',l''s''}{}^J\psi_{l''s'',ls}{}^J +\frac{l(l+1)}{r^2}\psi_{l's',ls}{}^J=k^2\psi_{l's',ls}{}^J. \quad (2.10)$$

If we are considering the scattering of particles with no spin then V and ψ are diagonal and equations (2.8) and (2.10) become uncoupled. If H_I is invariant under space reflection then the conservation of parity implies that for the scattering of a spin $\frac{1}{2}$ particle by a spin-zero particle, the equations are also uncoupled. In case both particles have spin $\frac{1}{2}$ it is the tensor force alone which couples them.

The amplitude $\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})$ for scattering from the initial momentum $\hbar\mathbf{k}$ and spin $\hbar s,\hbar\nu$ to the final momentum $\hbar\mathbf{k}'$ and spin $\hbar s',\hbar\nu'$ is defined by the asymptotic form of ψ for large r; thus

$$\psi_+(\mathbf{k}s\nu,\mathbf{r})\sim[(\mu k)^{\frac{1}{2}}/\hbar(2\pi)^{\frac{3}{2}}] \times[\chi_s{}^\nu e^{i\mathbf{k}\cdot\mathbf{r}}+r^{-1}e^{ikr}\sum_{s'\nu'}\chi_{s'}{}^{\nu'}\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})], \quad (2.11)$$

where $\mathbf{k}'=k\mathbf{r}r^{-1}$. Taking the limit of (2.2) for large r

[1] J. M. Blatt and V. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952).

leads by (2.3) to

$$\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})=-\frac{(2\pi)^2}{k}\int(d\mathbf{r})\psi_0^*(\mathbf{k}'s'\nu',\mathbf{r}) \times H_I(\mathbf{r})\psi_+(\mathbf{k}s\nu,\mathbf{r}). \quad (2.12)$$

If we expand in spherical harmonies according to (2.5) and (2.6), we obtain

$$\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k}) =-\frac{4\pi}{k^2}\sum_{JMll'mm'} i^{l-l'}Y_{l'}^{m'}(\mathbf{k}')C_{l's'}(J,M;m',\nu') \times Y_l^{m*}(\mathbf{k})C_{ls}(J,M;m,\nu)\sum_{l''s''}\int_0^\infty dr u_{l'}(kr) \times V_{l's',l''s''}^J(r)\psi_{l''s'',ls}^J(k,r). \quad (2.13)$$

The scattering matrix is defined as the probability amplitude for finding, at the time $t=+\infty$, momentum $\hbar\mathbf{k}'$ and spins $\hbar s'$, $\hbar\nu'$, if they were $\hbar\mathbf{k}$ and $\hbar s$, $\hbar\nu$ at the time $t=-\infty$.[2,3]

$$(\mathbf{k}'s'\nu'|S|\mathbf{k}s\nu) \equiv\lim_{t\to\infty}\int(d\mathbf{r})\psi_0^*(\mathbf{k}'s'\nu',\mathbf{r})e^{i(E'-E)t/\hbar}\psi_+(\mathbf{k}s\nu,\mathbf{r}) =\delta(E-E')[\delta(\Omega_k-\Omega_{k'})\delta_{ss'}\delta_{\nu\nu'}+(ik/2\pi)\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})] \equiv\delta(E-E')\sum_{JMll'mm'}Y_{l'}^{m'}(\mathbf{k}')Y_l^{m*}(\mathbf{k})i^{l-l'} \times C_{l's'}(J,M;m',\nu')C_{ls}(J,M;m,\nu)S_{l's',ls}^J(k), \quad (2.14)$$

where the second line follows from the integral equation (2.2) and (2.3). It follows from (2.12) that

$$\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})=-2\pi ik^{-1}\sum_{JMll'mm'}Y_{l'}^{m'}(\mathbf{k}')Y_l^{m*}(\mathbf{k}) \times C_{l's'}(J,M;m',\nu')C_{ls}(J,M;m,\nu)i^{l-l'} \times(S_{l's',ls}^J-\delta_{ll'}\delta_{ss'}). \quad (2.15)$$

Conservation of particles implies that S is unitary. It therefore follows from (2.15) that

$$-2\pi ik^{-1}[\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})-\Theta_{s\nu,s'\nu'}^*(\mathbf{k},\mathbf{k}')] =\sum_{s''\nu''}\int d\Omega_k''\Theta_{s''\nu'',s\nu}(\mathbf{k}'',\mathbf{k})\Theta_{s''\nu'',s'\nu'}^*(\mathbf{k}'',\mathbf{k}'). \quad (2.16)$$

A special case is the "optical theorem," which is obtained by setting $s=s'$, $\nu=\nu'$, $\mathbf{k}=\mathbf{k}'$[4]:

$$4\pi k^{-1}\,\mathrm{Im}\Theta_{s\nu,s\nu}(\mathbf{k},\mathbf{k})=\sum_{s'\nu'}\int d\Omega_{k'}|\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})|^2 =\sigma_{s\nu}^{\text{total}}(\mathbf{k}). \quad (2.16')$$

A further property of the S matrix follows if H_I is invariant under time reversal. We use a time-reversal operator[5] ϑ and spin functions and spherical harmonics such that

$$\vartheta\mathcal{Y}_{Jls}^M(\mathbf{r})=(-)^{J+M}\mathcal{Y}_{Jls}^{-M}(\mathbf{r}).$$

This is obtained by taking real χ and spherical harmonics which are such that[6]

$$Y_l^{m*}=(-)^{l+m}Y_l^{-m},$$

and the time-reversal operator

$$\vartheta=(i\sigma_y^{(1)})(i\sigma_y^{(2)})K,$$

$\sigma^{(1)}$ and $\sigma^{(2)}$ being the spin matrices for particles #1 and #2 (with $i\sigma_y=1$ if the particle has spin zero) and K, the antiunitary complex conjugation operator. The Clebsch-Gordan coefficients are such that

$$C_{ls}(J,-M;-m,-\nu)=(-)^{l+s-J}C_{ls}(J,M;m,\nu).$$

With these conventions we have

$$\vartheta\psi_0(\mathbf{k}s\nu,\mathbf{r})=(-)^{s+\nu}\psi_0(-\mathbf{k}s-\nu;\mathbf{r}),$$

and therefore, by (2.2),

$$\vartheta\psi_+(\mathbf{k}s\nu,\mathbf{r})=(-)^{s+\nu}\psi_-(-\mathbf{k}s-\nu,\mathbf{r}),$$

where ψ_- satisfies the integral equation (2.2) with $G_-=G_+^*$, the incoming wave Green's function.

It then follows from

$$(\psi_1,\psi_2)=(\vartheta\psi_2,\vartheta\psi_1)$$

and the assumed time-reversal invariance of H_I that the potential matrix of (2.9) is *symmetric:*

$$V_{ls,l's'}^J(r)=V_{l's',ls}^J(r). \quad (2.17)$$

Since H_I is Hermitian, $V_{ls,l's'}^J$ is consequently *real.* For the scattering amplitude, we get, from (2.12),

$$\Theta_{s'\nu',s\nu}(\mathbf{k}',\mathbf{k})=(-)^{s-s'+\nu-\nu'}\Theta_{s-\nu,s'-\nu'}(-\mathbf{k},-\mathbf{k}'), \quad (2.18)$$

which is the *reciprocity theorem.* It follows from (2.15) that it is equivalent to the *symmetry* of $S_{ls,l's'}^J$ as defined in (2.14):

$$S_{ls,l's'}^J=S_{l's',ls}^J. \quad (2.19)$$

S^J being unitary and symmetric, it can be diagonalized by an orthogonal real matrix U:

$$S_{ls,l's'}^J=\sum_\alpha U_{ls,\alpha}^J\exp(2i\delta_\alpha^J)U_{\alpha,l's'}^J, \quad (2.20)$$

where the δ_α^J are *real.*

Comparison of (2.13) with (2.15) gives us another expression for the S matrix:

$$S_{l's',ls}^J(k)=\delta_{ll'}\delta_{ss'}-2ik^{-1}\sum_{l''s''}\int_0^\infty dr u_{l'}(kr) \times V_{l's',l''s''}^J(r)\psi_{l''s'',ls}^J(k,r). \quad (2.21)$$

[2] J. Jauch and F. Rohrlich, *Theory of Photons and Electrons* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1955).

[3] C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. 23, No. 1 (1945).

[4] We write Re A and Im A for the real and imaginary parts of A.

[5] E. P. Wigner, *Group Theory* (Academic Press, Inc., New York, 1959), p. 325 ff.

[6] Those of Blatt and Weisskopf,[1] say, multiplied by i^l; see footnote 5, p. 345, of E. P. Wigner.[5]

We may now identify S^J by the asymptotic form of the radial wave function. In order to do that we require the asymptotic values of the Riccatti-Bessel functions for large r:

$$\begin{aligned} u_l(kr) &\sim \sin(kr-\tfrac{1}{2}\pi l), \\ v_l(kr) &\sim -\cos(kr-\tfrac{1}{2}\pi l), \\ w_l(kr) &\sim i^l e^{-ikr}. \end{aligned} \tag{2.22}$$

Equation (2.8) together with (2.4) and (2.21) shows that as $r\to\infty$,

$$\psi_{ls,l's'}{}^J(k,r) \sim \tfrac{1}{2}i^{l+1}[\delta_{ll'}\delta_{ss'}e^{-ikr}-(-)^l e^{ikr}S_{ls,l's'}{}^J(k)], \tag{2.23}$$

and therefore, by (2.20),

$$\begin{aligned} \psi_{ls,\alpha}{}^J(k,r) &\equiv \sum_{l's'} \psi_{ls,l's'}{}^J(k,r)U_{l's',\alpha}{}^J(k) \\ &\sim U_{ls,\alpha}{}^J(k)\exp[i\delta_\alpha{}^J(k)]\sin(kr-\tfrac{1}{2}\pi l+\delta_\alpha{}^J). \end{aligned} \tag{2.24}$$

Thus $\delta_\alpha{}^J(k)$ is identified as the eigenphaseshift. The characteristic property of $\psi_{ls,\alpha}{}^J$ is that all its components experience the same phaseshift.

We want to investigate the properties of solutions of the radial equation (2.10). In Secs. 3 to 8 we restrict ourselves to the case of no coupling, which is realized when one of the particles has spin zero and the other, spin less than two (provided H_I conserves parity); or else if both have spin $\frac{1}{2}$, but tensor forces are neglected.

If there is no coupling; i.e., the matrix V^J is diagonal, then only one subscript, l, will be used everywhere, that being the only index on which Eq. (2.10) explicitly depends via the centrifugal term.

3. REGULAR AND IRREGULAR SOLUTIONS

We return to the radial equation (2.10) in the case of no coupling. Rather than considering the "physical" solution ψ_l we define regular and irregular solutions by boundary conditions which lead to simple properties as functions of k.

The weakest assumptions we shall ever make concerning the potential are the existence of its first and second absolute moments:

$$\int_0^\infty dr r|V(r)|<\infty, \tag{3.1a}$$

$$\int_0^\infty dr r^2|V(r)|<\infty. \tag{3.1b}$$

Whenever stronger assumptions are made they will be stated explicitly.

Hypothesis (3.1a) implies that V behaves better than r^{-2} near the origin. There exists consequently a regular solution $\varphi_l(k,r)$ of (2.10) which near $r=0$ behaves like $u_l(kr)$. As $kr\to 0$ we have[7]

$$\begin{aligned} u_l(kr) &= (kr)^{l+1}/(2l+1)!!+O[(kr)^{l+3}], \\ v_l(kr) &= -(kr)^{-l}(2l-1)!!+O[(kr)^{-l+2}]. \end{aligned} \tag{3.2}$$

We therefore define $\varphi_l(k,r)$ by the boundary condition

$$\lim_{r\to 0}(2l+1)!!r^{-l-1}\varphi_l(k,r)=1. \tag{3.3}$$

It then follows immediately that $\varphi_l(k,r)$ is a function of k^2 only and that for real k it is real.

Hypothesis (3.1b) implies that at infinity V behaves better than r^{-3} so that a Coulomb field, for example, is excluded. It follows (as will be shown later) that at infinity all solutions of (2.10) oscillate like sine or cosine waves. It is then convenient to define another solution $f_l(k,r)$ by the boundary condition

$$\lim_{r\to\infty} e^{ikr}f_l(k,r)=i^l. \tag{3.4}$$

This function does not vanish at $r=0$, in general, but it is $O(r^{-l})$ there, as is $w_l(kr)$. It follows immediately from the boundary condition (3.4) and from the reality of the differential equation (2.10) that for real k

$$f_l{}^*(-k,r)=(-)^l f_l(k,r). \tag{3.5}$$

We now want to extend all our definitions to complex values of k. It then follows from the k independence of the boundary condition[8] (3.3) that for fixed r, $\varphi_l(k,r)$ is an analytic function of k regular for all finite values of k; i.e., an entire function of k. The function $f_l(k,r)$ is for fixed $r>0$ an analytic function of k regular in the open lower half of the complex k plane; in the upper half of the k plane it may be expected to have singularities since (3.4) is not sufficient there to define $f_l(k,r)$ uniquely. These statements are intended merely as a guide and will be proved later.

It is clear that in any region of analyticity connected with the real axis Eq. (3.5) implies

$$f_l{}^*(-k^*,r)=(-)^l f_l(k,r). \tag{3.5'}$$

We can readily replace the differential equation (2.10) and boundary conditions (3.3) or (3.4) by integral equations. If we define

$$\begin{aligned} g_l(k;r,r') &\equiv k^{-1}[u_l(kr')v_l(kr)-u_l(kr)v_l(kr')] \\ &= i(-)^l(2k)^{-1}[w_l(kr)w_l(-kr')-w_l(-kr)w_l(kr')], \end{aligned} \tag{3.6}$$

[7] We use the following notation: "$f(x)=O(x)$ as $x\to\infty$ (or 0)" means that $f(x)/x$ is bounded as $x\to\infty$ (or 0); "$f(x)=o(x)$ as $x\to\infty$ (or 0)" means that $f(x)/x$ tends to naught as $x\to\infty$ (or 0).

[8] According to a theorem by Poincaré the solution of an ordinary linear differential equation containing an entire function of a parameter k, defined by a boundary condition independent of k, is itself an entire function of k. See footnote reference 9; also see footnote 8 of Jost and Pais.[10] We shall use this theorem as a guidance only and prove it for the special case of $\varphi_l(k,r)$.

[9] E. Hilb, *Encycl. der Math. Wissensch.* (B. G. Teubner, Leipzig, 1915), Vol. 2, Part 2, p. 501.

[10] R. Jost and A. Pais, Phys. Rev. 82, 840 (1951).

then

$$G_l^{(1)}(k;r,r')=\begin{cases} g_l(k;r,r'), & r'\leq r, \\ 0, & r'\geq r, \end{cases}$$

is a Green's function [compare with (2.4)] and so is

$$G_l^{(2)}(k;r,r')=\begin{cases} 0, & r'\leq r, \\ -g_l(k;r,r'), & r'\geq r. \end{cases}$$

The first is appropriate to the definition of φ_l and the second, to that of f_l; thus

$$\varphi_l(k,r)=k^{-l-1}u_l(kr) + \int_0^r dr' g_l(k;r,r')V(r')\varphi_l(k,r'), \quad (3.7)$$

$$f_l(k,r)=w_l(kr)-\int_r^\infty dr' g_l(k;r,r')V(r')f_l(k,r'). \quad (3.8)$$

The existence and analytic properties of φ_l and f_l are proved by means of these integral equations. Their advantage over the integral equation (2.8) for the physical wave function ψ_l is that they can be solved by successive approximations, provided only that V satisfies (3.1), irrespective of its *strength*. The reason is that the integrations run from naught to r only, or from r to infinity.

In order to prove the convergence[11] of the sequence of successive approximations, one uses the following bounds, true in the entire complex plane[16]

$$\begin{aligned} |u_l(kr)| &\leq Ce^{|\nu|r}[L(|k|r)]^{l+1}, \\ |v_l(kr)| &\leq Ce^{|\nu|r}[L(|k|r)]^{-l}, \\ |w_l(kr)| &\leq Ce^{\nu r}[L(|k|r)]^{-l}, \end{aligned} \quad (3.9)$$

where $\nu\equiv \mathrm{Im}k$ and

$$L(x)\equiv x/(1+x).$$

It is then easily seen that for $r'\leq r$

$$\begin{aligned} |g_l(k;r,r')| &= |g_l(k;r',r)| \\ &\leq Ce^{|\nu|(r-r')}|k|^{-1}[L(|k|r)]^{l+1}[L(|k|r')]^{-l}. \end{aligned} \quad (3.10)$$

We now solve (3.7) by successive approximation:

$$\varphi_l(k,r)=\sum_0^\infty \varphi_l^{(n)}(k,r),$$

where

$$\varphi_l^{(0)}(k,r)=k^{-l-1}u_l(kr)$$

$$\varphi_l^{(n)}(k,r)=\int_0^r dr' g_l(k;r,r')V(r')\varphi_l^{(n-1)}(k,r'), \quad n\geq 1.$$

If we use (3.10), we get

$$\begin{aligned} |\varphi_l^{(n)}(k,r)| \leq C\int_0^r dr' e^{|\nu|(r-r')}|k|^{-1}[L(|k|r)]^{l+1} \\ \times[L(|k|r')]^{-l}|V(r')||\varphi_l^{(n-1)}(k,r')|. \end{aligned}$$

Now writing for the moment,

$$\mathfrak{A}_l^{(n)}(k,r)\equiv \varphi_l^{(n)}(k,r)e^{-|\nu|r}|k|^{l+1}[L(|k|r)]^{-l-1},$$

we have

$$|\mathfrak{A}_l^{(0)}(k,r)|\leq C$$

$$\begin{aligned} |\mathfrak{A}_l^{(n)}(k,r)| \leq C\int_0^r dr' |\mathfrak{A}_l^{(n-1)}(k,r')| \\ \times|V(r')|L(|k|r')|k|^{-1}, \quad n\geq 1, \end{aligned}$$

and therefore

$$\begin{aligned} |\mathfrak{A}_l^{(n)}(k,r)| &\leq C^{n+1}\int_0^r dr_1\cdots\int_0^{r_{n-1}} dr_n|V(r_1)| \\ &\times\frac{r_1}{1+|k|r_1}\cdots|V(r_n)|\frac{r_n}{1+|k|r_n} \\ &=\frac{C^{n+1}}{n!}\left[\int_0^r dr'|V(r')|\frac{r'}{1+|k|r'}\right]^n, \end{aligned}$$

so that

$$|\sum_0^\infty \mathfrak{A}_l^{(n)}(k,r)|\leq C\exp\left[C\int_0^r dr'|V(r')|r'(1+|k|r')^{-1}\right].$$

As a result the series $\sum\varphi_l^{(n)}$ converges absolutely and uniformly for all r and in every finite region in the complex k plane. Furthermore, we find that

$$\begin{aligned} |\varphi_l(k,r)| \leq Ce^{|\nu|r}\left(\frac{r}{1+|k|r}\right)^{l+1} \\ \times\exp\left[C\int_0^r dr'|V(r')|\frac{r'}{1+|k|r'}\right]. \end{aligned} \quad (3.11)$$

Since g_l and $\varphi_l^{(0)}$ are entire analytic functions of k, so is each $\varphi_l^{(n)}$. It then follows that for every fixed r, $\varphi_l(k,r)$ is an entire function of k^2.

We may now insert (3.11) in the integral equation (3.7) and obtain the inequality

$$\begin{aligned} |\varphi_l(k,r)-k^{-l-1}u_l(kr)| \\ \leq Ce^{|\nu|r}\left(\frac{r}{1+|k|r}\right)^{l+1}\int_0^r dr'|V(r')|\frac{r'}{1+|k|r'}. \end{aligned} \quad (3.12)$$

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[11] The procedure below follows Jost[12] and Levinson.[13] It can be generalized to certain restricted nonlocal potentials; see Martin.[14,15]

[12] R. Jost, Helv. Phys. Acta **20**, 256 (1947).

[13] N. Levinson, Kgl. Danske Videnskab. Selskab., Mat.-fys. Medd. **25**, No. 9 (1949).

[14] A. Martin, Compt. rend. **243**, 22 (1956).

[15] A. Martin, Nuovo cimento **14**, 403 (1959).

[16] The first inequality was given by Levinson,[13] the others by Newton.[17]

[17] R. G. Newton, Phys. Rev. **100**, 412 (1955).

The integral on the right-hand side tends to naught as $|k| \to \infty$, even if at $r=0$ only the first moment of $|V|$ exists. That is seen by writing

$$\int_0^\infty dr|V(r)|\frac{r}{1+|k|r}=\int_0^a+\int_a^\infty \leq \int_0^a drr|V(r)| + \int_a^\infty dr|V(r)||k|^{-1}.$$

Hence if we choose a and k so that

$$\int_0^a drr|V(r)| \leq \tfrac{1}{2}\epsilon, \quad |k| \geq \int_a^\infty dr|V(r)|\cdot 2\epsilon^{-1}$$

then

$$\int_0^\infty dr|V(r)|r(1+|k|r)^{-1} \leq \epsilon.$$

The right-hand side of (3.12) is therefore

$$o(|k|^{-l-1}e^{|\nu|r}) \quad \text{as} \quad |k| \to \infty,$$

and consequently, as $|k| \to \infty$

$$\varphi_l(k,r)=k^{-l-1}\sin(kr-\tfrac{1}{2}\pi l)+o(|k|^{-l-1}e^{|\nu|r}) \quad (3.13)$$

uniformly in r. It is clear from (3.12) that if V is absolutely integrable, then the remainder is $O(|k|^{-l-2}e^{|\nu|r})$.

A similar procedure is followed for the function $f_l(k,r)=\sum f_l^{(n)}(k,r)$, where

$$f_l^{(0)}(k,r)=w_l(kr)$$

$$f_l^{(n)}(k,r)=-\int_r^\infty dr' g_l(k;r,r')V(r')f_l^{(n-1)}(k,r'), \quad n \geq 1.$$

One then finds that the series $\sum h_l^{(n)}(k,r)$, where

$$h_l^{(n)}(k,r)\equiv e^{-\nu r}[L(|k|r)]^l f_l^{(n)}(k,r),$$

is dominated by a series which can be summed to

$$C\exp\Big[C\int_r^\infty dr'|V(r')| \times \exp[(\nu+|\nu'|)(r'-r)]r'(1+|k|r')^{-1}\Big].$$

The series $\sum f_l^{(n)}$ therefore converges uniformly for all $r \geq r_0>0$ and for any closed region in the complex k plane not including $k=0$, where

$$\alpha \equiv \int_0^\infty dr|V(r)|re^{(\nu+|\nu|)r}$$

is finite. Thus $f_l(k,r)$ exists, is continuous, and is obtainable by successive approximations from (3.8) for all $r>0$ and all finite $k \neq 0$ in the lower half-plane, including the real axis, provided only that V possesses a finite first absolute moment. If, moreover, V decreases exponentially at infinity so that

$$\int_0^\infty drr|V(r)|e^{2ar}<\infty \quad (3.14)$$

for some $a>0$, then it follows that $f_l(k,r)$ exists and is continuous (and is obtainable by successive approximations) in a strip in the upper half of the complex k plane with $\mathrm{Im}k \leq a$, except at $k=0$.

We also get the inequality

$$|f_l(k,r)| \leq Ce^{\nu r}[(1+|k|r)/|k|r]^l e^{Ca}, \quad (3.15)$$

which inserted in (3.8) yields

$$|f_l(k,r)-w_l(kr)| \leq Ce^{\nu r}\left(\frac{1+|k|r}{|k|r}\right)^l \times e^{Ca}\int_r^\infty dr'|V(r')|e^{(\nu+|\nu|)(r'-r)}\frac{r'}{1+|k|r'}. \quad (3.16)$$

By the same argument that follows (3.12) the right-hand side of (3.16) is $o(e^{\nu r})$ as $|k| \to \infty$ uniformly for all $r \geq r_0>0$ in the lower half of the complex k plane including the real axis, and in a strip of width a in the upper half-plane if (3.14) holds. Therefore, as $|k| \to \infty$

$$f_l(k,r)=i^l e^{-ikr}+o(e^{\nu r}). \quad (3.17)$$

The inequality (3.16) also shows that

$$\lim_{k\to 0} k^l f_l(k,r)$$

exists for all finite $r>0$ if the limit is carried out in the region of regularity.

In order to show that $f_l(k,r)$ is an analytic function of k we must show the existence and continuity of its first derivative with respect to k in the same manner as those of $f_l(k,r)$ itself. (Since the integral in (3.8) converges absolutely, differentiation under the integral sign is permitted.) We cannot use the same argument here as for $\varphi_l(k,r)$ because $f_l^{(n)}$ is not necessarily regular. The result is that, provided V has a finite second absolute moment, $f_l(k,r)$ for fixed $r>0$ is an analytic function of k regular everywhere in the open lower half of the complex plane and continuous on the real axis, except at $k=0$. If the potential satisfies (3.14) then the region of regularity includes a strip in the upper half-plane up to $\mathrm{Im}k<a$, except for a pole of order l at $k=0$. If the potential vanishes identically outside a finite region, then $k^l f_l(k,r)$ is an entire function of k for all fixed $r>0$.

If the potential satisfies (3.14) then one may obtain information about the singularities of $f_l(k,r)$ for $\mathrm{Im}k \geq a$ in a relatively simple way.[18] If we write

$$f_l(k,r)\equiv f_l^{(0)}(k,r)+\chi_l^{(1)}(k,r),$$

where $f_l^{(0)}(k,r)=w_l(kr)$, then $\chi_l^{(1)}$ satisfies the integral

[18] T. Regge, Nuovo Cimento 9, 295 (1958).

equation

$$\chi_l^{(1)}(k,r)=f_l^{(1)}(k,r)-\int_r^\infty dr' g_l(k;r,r')V(r')\chi_l^{(1)}(k,r'),$$

where $f_l^{(1)}$ is simply the first Born approximation:

$$f_l^{(1)}(k,r)=-\int_r^\infty dr' g_l(k;r,r')V(r')w_l(kr').$$

Suppose that for a given V this integral is carried out and it admits an analytic continuation into a region in the upper half-plane with $\mathrm{Im}k\geq a$, and we can set there

$$|f_l^{(1)}(k,r)|\leq Ce^{\gamma r}.$$

We may then use this inequality in place of (3.9) and prove the analyticity of $\chi_l^{(1)}$ by the same arguments which prove it for f_l. The result is evidently that $\chi_l^{(1)}(k,r)$ is regular where $f_l^{(1)}(k,r)$ is in the region $\mathrm{Im}k<2a-\gamma$. If, for example, $\gamma=\nu-2a$ as it is for $\mathrm{Im}k<a$, then the continuation works for $\mathrm{Im}k=\nu<2a$. One may repeat the same argument by examining explicitly the analytic continuation of the second Born approximation $f_l^{(2)}$, and thus extend the strip of analyticity further and further, except for explicitly isolated singularities.

4. JOST FUNCTION $f_l(k)$

The functions $f_l(k,r)$ and $f_l(-k,r)$ are two linearly independent solutions (for $k\neq 0$) of the differential equation (2.10). The regular solution $\varphi_l(k,r)$ can therefore be expressed as a linear combination of them. Since $\varphi_l(k,r)$ is even in k this defines a function $f_l(k)$, so that[12]

$$\varphi_l(k,r)=\tfrac{1}{2}ik^{-l-1}\times[f_l(-k)f_l(k,r)-(-)^l f_l(k)f_l(-k,r)]. \quad (4.1)$$

We want to get a more explicit equation for $f_l(k)$. That can be obtained by taking the Wronskian of $\varphi_l(k,r)$ and $f_l(k,r)$. The Wronskian of two solutions of the same linear second-order differential equation being independent of r, we readily find, by evaluating it at $r\to\infty$ and using the boundary condition (3.4) that

$$W[f_l(k,r),f_l(-k,r)]=(-)^l 2ik,$$

where

$$W[f,g]\equiv fg'-f'g. \quad (4.2)$$

If we make use of this and (4.1), we obtain

$$f_l(k)=k^l W[f_l(k,r),\varphi_l(k,r)]. \quad (4.3)$$

Because of the boundary condition (3.3) this implies that

$$f_l(k)=\lim_{r\to 0}(kr)^l f_l(k,r)/(2l-1)!!. \quad (4.3')$$

If we insert the integral equations (3.7) and (3.8) in (4.3) and evaluate it at $r=0$ or $r=\infty$, we obtain the following two integral representations for $f_l(k)$:

$$f_l(k)=1+k^{-l}\int_0^\infty dr f_l(k,r)V(r)u_l(kr)$$

$$=1+k^l\int_0^\infty dr\varphi_l(kr)V(r)w_l(kr). \quad (4.4)$$

We may now express the S matrix in terms of $f_l(k)$. The asymptotic form for large r of $\varphi_l(k,r)$ follows immediately from (4.1) and the boundary condition (3.4); thus

$$\varphi_l(k,r)\sim\tfrac{1}{2}i^{l+1}k^{-l-1}\times[f_l(-k)e^{-ikr}-(-)^l f_l(k)e^{ikr}]. \quad (4.1')$$

Comparison with (2.23) shows that

$$S_l(k)=f_l(k)/f_l(-k). \quad (4.5)$$

It follows that

$$S_l(-k)=1/S_l(k). \quad (4.6)$$

Furthermore, φ_l being real and even in k it follows from (3.5) and (4.3) that for real k

$$f_l^*(-k)=f_l(k), \quad (4.7)$$

and, consequently,

$$|S_l(k)|=1.$$

This is the unitarity condition.

The relation between φ_l and the physical wave function ψ_l is provided by a comparison of (4.1′) with (2.23); thus

$$\psi_l(k,r)=[k^{l+1}/f_l(-k)]\varphi_l(k,r). \quad (4.8)$$

This furnishes the physical significance of the function $f_l(k)$. Equation (4.5) together with (4.7) and (2.20) shows that

$$f_l(k)=|f_l(k)|\exp[i\delta_l(k)], \quad (4.9)$$

where δ_l is the *phaseshift* for the lth partial wave, while (4.8) with (3.3) shows that

$$|\psi_l(k,r)|^2\underset{r\to 0}{\longrightarrow}|\psi_l^{(0)}(k,r)|^2/|f_l(k)|^2,$$

$\psi_l^{(0)}$ being the wave function in the absence of a potential. Thus the phase of $f_l(k)$ is the lth phaseshift and the inverse of the square of its modulus measures the probability of finding the particles in each other's proximity relative to what it would be in the absence of forces between them.

The Jost function $f_l(k)$ may also be approached from quite a different point of view. Suppose that one were to solve the integral equation (2.8) for the physical wave function by the Fredholm method.[10,19] One would then have to form the Fredholm determinant

$$\Delta_l(k)=1+\sum_{n=1}^\infty\frac{(-)^n}{n!}\int_0^\infty dr_1\cdots\int_0^\infty dr_n \times V(r_1)\cdots V(r_n)D_l(k;r_1,\cdots,r_n),$$

where

$$D_l(k;r_1,\cdots,r_n)=\begin{vmatrix} G_l(k;r_1,r_1) & G_l(k;r_1,r_2)\cdots \\ G_l(k;r_2,r_1) & G_l(k;r_2,r_2)\cdots \\ \vdots & \end{vmatrix}.$$

$G_l(k;r,r')$ being given by (2.4). Because the integrand in $\Delta_l(k)$ is symmetric in $r_1,\cdots,r_n$, and because

[19] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, New York, 1948), p. 211 ff.

of the symmetry properties of the spherical Bessel functions we can write

$$\Delta_l(-k)=1+\sum_1^\infty k^{-n}\int_0^\infty dr_1\int_0^{r_1}dr_2\cdots\int_0^{r_{n-1}}dr_n \times V(r_1)\cdots V(r_n)d_l(k;r_1,\cdots,r_n) \quad (4.10)$$

with

$$d_l(k;r_1,\cdots,r_n)=\begin{vmatrix} w_l(kr_1)u_l(kr_1) & w_l(kr_1)u_l(kr_2)\cdots w_l(kr_1)u_l(kr_n)\\ w_l(kr_1)u_l(kr_2) & w_l(kr_2)u_l(kr_2)\cdots w_l(kr_2)u_l(kr_n)\\ \vdots & \\ w_l(kr_1)u_l(kr_n) & w_l(kr_2)u_l(kr_n)\cdots w_l(kr_n)n_l(kr_n)\end{vmatrix} \equiv w_l(kr_1)s_l(k;r_1;r_2,\cdots,r_n).$$

Consequently,

$$\Delta_l(-k)=1+k^{-1}\int_0^\infty dr w_l(kr)V(r)g_l(kr), \quad (4.11)$$

where

$$g_l(k,r)=u_l(kr)+\sum_1^\infty k^{-n}\int_0^r dr_1\int_0^{r_1}dr_2\cdots\int_0^{r_{n-1}}dr_n \times V(r_1)\cdots V(r_n)s_l(k;r;r_1,\cdots,r_n).$$

Now since $s_l(k;r;r,r_2,\cdots,r_n)=0$ and

$$W[w_l(kr),u_l(kr)]=k,$$

we readily find that

$$W[w_l(kr),g_l(k,r)]=k\Big[1+\sum_1^\infty k^{-n}\int_0^r dr_1\cdots\int_0^{r_{n-1}}dr_n \times V(r_1)\cdots V(r_n)d_l(k;r_1,\cdots,r_n)\Big]. \quad (4.12)$$

Differentiation with respect to r yields

$$w_l(kr)g_l''(k,r)-g_l(k,r)w_l''(kr)=kw_l(kr)V(r)g_l(k,r),$$

which, because of the differential equation satisfied by $w_l(kr)$, shows that $g_l(k,r)$ solves the differential equation (2.10). Furthermore one easily sees from (4.12) that as $r\to 0$,

$$g_l(k,r)=u_l(kr)+o(r^{l+1}).$$

It follows that

$$g_l(k,r)=k^{l+1}\varphi_l(k,r), \quad (4.13)$$

and therefore by (4.11) and (4.3),

$$f_l(k)=\Delta_l(-k). \quad (4.14)$$

Thus the function $f_l(-k)$ is the Fredholm determinant of Eq. (2.8).[10]

We now want to examine the analytic properties of $f_l(k)$ in the complex plane; that will, via (4.5), give us information on the analytic properties of the S matrix.

In order to extend $f_l(k)$ into the complex plane we may use either (4.3) or (4.4). The inequalities (3.9) and (3.11) lead from the second version of (4.4) to

$$|f_l(k)-1|\le C\int_0^\infty dr|V(r)|e^{(\nu+|\nu|)r}r(1+|k|r)^{-1}. \quad (4.15)$$

Under the assumptions (3.1) on the potential, the integral thus converges absolutely so that $f_l(k)$ exists and is continuous for all k in the closed lower half-plane. If the potential also satisfies (3.14) then the same conclusion can be drawn in an additional strip in the upper half-plane with $\mathrm{Im}k\le a$. Because of the absolute convergence we may differentiate (4.4) with respect to k under the integral sign and then use inequalities obtained from differentiating (3.8) with respect to k. The result is that under the hypothesis (3.1) $f_l(k)$ is an analytic function of k regular in the open lower half of the complex plane and continuous on the real axis. If the potential fulfills (3.14) then $f_l(k)$ is analytic also in a strip in the upper half-plane with $\mathrm{Im}k<a$. If the potential vanishes asymptotically faster than *every* exponential (e.g., if it has a gaussian tail or if it vanishes identically beyond a finite radius) then $f_l(k)$ is an entire function of k. In any region of analyticity connected with the real axis (4.7) leads to

$$f_l^*(-k^*)=f_l(k). \quad (4.7')$$

The arguments at the end of Sec. 3, which in specific cases of (3.14) may allow the analytic continuation of $f_l(k,r)$ beyond $\mathrm{Im}k=a$ by examination of the terms in the successive approximations,[18] are now applicable to $f_l(k)$. It may thus be possible in many practical cases to use the first Born approximation in order to extend the analytic continuation to $\mathrm{Im}k<2a$, the second, to $\mathrm{Im}k<3a$, etc.

We now want to examine the behavior of $f_l(k)$ as $k\to\infty$. The inequality (4.15) tells us directly that for $\mathrm{Im}k\le 0$,

$$\lim_{|k|\to\infty} f_l(k)=1. \quad (4.16)$$

In fact we can conclude from (4.3), (3.17), and (2.22) that when $\mathrm{Im}k\le 0$, as $|k|\to\infty$,

$$f_l(k)=1+(2ik)^{-1}\int_0^\infty drV(r)+o(k^{-1}), \quad (4.16')$$

provided that $V(r)$ is integrable at $r=0$; otherwise the second term need be only $o(1)$. Equation (4.16') says that at very high energies the Born approximation for $f_l(k)$ is good.[20]

In the upper half-plane we can draw interesting conclusions only if for $r>R$ the potential vanishes identi-

[20] The analyticity properties of $f_l(k)$ together with (4.7) and (4.16) imply, of course, that $f_l(k)$ satisfies a simple "dispersion relation" obtainable immediately from Cauchy's theorem. This was pointed out explicitly by Giambiagi and Kibble,[21] but it does not appear to have any useful application.

[21] J. J. Giambiagi and T. W. B. Kibble, Ann. Phys. 7, 39 (1959).

cally. In that event (4.15) shows that

$$|(f_l(k)-1)e^{2ikR}| \leq C\int_0^R dr\,|V(r)|\,r(1+|k|r)^{-1}.$$

This implies that for $\mathrm{Im}k>0$

$$(f_l(k)-1)e^{2ikR}=o(1) \quad \text{as} \quad |k|\to\infty \qquad (4.17)$$

if the potential has a finite first absolute moment; if it is also absolutely integrable then the right-hand side of (4.17) is $O(|k|^{-1})$.

Next we want to look at the zeros of $f_l(k)$. Suppose that $f_l(k)$ vanishes at a point in the lower half-plane:

$$f_l(k_0)=0, \quad \mathrm{Im}k_0<0.$$

Since by (4.3) this means that the Wronskian between $f_l(k_0,r)$ and $\varphi_l(k_0,r)$ is zero, the two solutions are multiples of one another:

$$f_l(k_0,r)=c\varphi_l(k_0,r). \qquad (4.18)$$

But k_0 being in the lower half-plane, the left-hand side of (4.18) decreases exponentially at infinity, while the right-hand side vanishes at the origin. Consequently, both sides are square integrable and k_0^2 is a discrete eigenvalue of the Schrödinger equation; there is a bound state of energy $\hbar^2k_0^2/2\mu$.

It is proved by the standard method that the eigenvalues k_0^2 must be real. If k_0 is a root of $f_l(k)$ in the lower half-plane, then by (4.7′), so is $-k_0^*$. Multiplication of the Schrödinger equation for $\varphi_l(k,r)$ by $\varphi_l(k',r)$ and subtraction from that for $\varphi_l(k',r)$ multiplied by $\varphi_l(k,r)$ leads to

$$(d/dr)W[\varphi_l(k,r),\varphi_l(k',r)] = (k^2-k'^2)\varphi_l(k,r)\varphi_l(k',r). \qquad (4.19)$$

If we now set $k=k_0$, $k'=-k_0^*$ and integrate from $r=0$ to $r=\infty$, we get

$$\mathrm{Im}k_0^2\int_0^\infty dr\,|\varphi_l(k_0,r)|^2=0$$

and therefore k_0^2 must be real.

The converse is also true. If k_0^2 is a discrete eigenvalue then $f_l(k_0,r)$ must vanish at $r=0$ when k_0 is taken in the lower half plane. Hence by (4.3′) $f_l(k_0)=0$.

If $k_0=-i\kappa$, $\kappa>0$, is a root of $f_l(k)$ and $k=i\kappa$ lies in a region of analyticity of $f_l(k)$ connected with the real axis, then Eq. (4.1) at once yields the following value for the constant c of (4.18):

$$c=-2i^{-l}\kappa^{l+1}/f_l(i|\kappa|). \qquad (4.20)$$

In general, however, we cannot draw this conclusion.

The function $f_l(k)$ cannot have any roots on the real axis, except possibly at $k=0$. That follows at once from the fact that by (4.7) $f_l(-k)$ vanishes when $f_l(k)$ does for real k. Equation (4.1) then shows that $\varphi_l(k,r)$ would vanish identically in r. Since that contradicts the boundary condition (3.3), $f_l(k)$ cannot vanish for real $k\neq 0$.

It is possible for $f_l(k)$ to be zero for $k=0$. We then conclude that the function

$$h_l(k,r)\equiv k^l f_l(k,r)$$

is, for $k=0$, a multiple of $\varphi_l(0,r)$

$$h_l(0,r)=c\varphi_l(0,r). \qquad (4.18')$$

For $l=0$, however, the boundary condition (3.4) shows that $h_l(0,r)$ is different from zero at $r=\infty$ so that $\varphi_l(0,r)$ is not normalizable and $k=0$ is not a discrete eigenvalue. For $l>0$, on the other hand, the inequality (3.15) shows that as $r\to\infty$,

$$h_l(0,r)=O(r^{-l});$$

$\varphi_l(0,r)$ is therefore square integrable and zero is a discrete eigenvalue if $f_l(0)=0$. We then have a zero energy-bound state. For $l=0$ this can happen only if the potential fails to satisfy (3.1); see Sec. 10f for an example.

The next question is naturally the multiplicity of the zeros of $f_l(k)$. Take first the case for which $f_l(k_0)=0$ with $\mathrm{Im}k_0<0$. Differentiation of (4.3) with respect to k (indicated by a dot), subsequently setting $k=k_0$ and using (4.18) leads to

$$\dot f_l(k_0)=k_0{}^l c^{-1}W[\dot f_l(k_0,r),f_l(k_0,r)] + k_0{}^l cW[\varphi_l(k_0,r),\dot\varphi_l(k_0,r)]. \qquad (4.21)$$

The right-hand side can be evaluated by differentiating (4.19) and the equivalent equation for $f_l(k,r)$ with respect to k, then setting $k=k_0$. The result is that if $f_l(k_0)=0$, then

$$\dot f_l(k_0)=-2k_0{}^{l+1}\left[c\int_0^r dr'\,\varphi_l^2(k_0,r')+c^{-1}\int_r^\infty dr' f_l^2(k_0,r')\right]$$

$$=-2ck_0{}^{l+1}\int_0^\infty dr\,\varphi_l^2(k_0,r). \qquad (4.21')$$

Because of the boundary condition (3.4), $c\neq 0$; furthermore, $\varphi_l(k_0,r)$ is real for purely imaginary k_0; hence the right-hand side of (4.21′) cannot vanish. Consequently, $\dot f_l(k_0)\neq 0$ when $f_l(k_0)=0$ and the zero is *always simple.*

The point $k=0$ requires special consideration. Suppose that $f_l(0)=0$. We then take k first in the lower half-plane, $\mathrm{Im}k<0$, and differentiate the equivalent of (4.19) for $h_l(k,r)$ with respect to k, subsequently setting $k'=k$:

$$W[\dot h_l(k,r),h_l(k,r)]=-2k\int_r^\infty dr'h_l^2(k,r'). \qquad (4.22)$$

The next step is to let k tend to naught inside a cone of opening angle less than π:

$$-\mathrm{Im}k\geq\epsilon|k|, \quad \epsilon>0.$$

It is then easily shown by means of the inequalities (3.16), (3.15), and (3.9) that the right-hand side of

(4.22) has the same limit with $k \to 0$ as

$$\lim_{k\to 0} 2k \int_r^\infty dr' w_l^2(kr') k^{2l}$$
$$= 2 \lim \left[k^{2l} \int_{kr}^a dz w_l^2(z) + k^{2l+1} \int_{a/k}^\infty dr' e^{-2ikr'} i^{2l} \right]$$
$$= \begin{cases} 0, & \text{if } l \geq 1, \\ -i, & \text{if } l = 0. \end{cases}$$

As a result, (4.22) leads to

$$W[\dot{h}_l(0,r), h_l(0,r)] = \begin{cases} 0, & \text{if } l \geq 1, \\ i, & \text{if } l = 0, \end{cases} \tag{4.23}$$

when $k=0$ is approached as indicated. Equation (4.21) for $k_0=0$ reads

$$\dot{f}_l(0) = c^{-1} W[\dot{h}_l(0,r), h_l(0,r)] + cW[\varphi_l(0,r), \dot{\varphi}_l(0,r)], \tag{4.21''}$$

where we may let r tend to zero. Equation (4.23) thus shows that if $f_l(0)=0$, then

$$\dot{f}_l(0) = \begin{cases} ic^{-1}, & \text{if } l = 0, \\ 0, & \text{if } l \geq 1. \end{cases} \tag{4.24}$$

For $l \geq 1$ one further differentiation is required. Since then $\dot{f}_l(0)=0$, we have from (4.21) and (4.22)

$$\ddot{f}_l(0) = \lim_{k\to 0} k^{-1} \dot{f}_l(k) = -2c \int_0^\infty dr \varphi_l^2(0,r). \tag{4.21'''}$$

We therefore find that if $f_l(0)=0$, then as $k \to 0$ with $-\mathrm{Im}k \geq \epsilon |k|$, $\epsilon > 0$,

$$1/f_l(k) = \begin{cases} O(k^{-1}), & \text{if } l = 0, \\ O(k^{-2}), & \text{if } l \geq 1, \end{cases} \tag{4.25}$$

as well as

$$f_l(k) = \begin{cases} O(k), & \text{if } l = 0, \\ O(k^2), & \text{if } l \geq 1, \end{cases} \tag{4.25'}$$

which is to say that f_l goes to zero *exactly* as k or k^2, respectively. If $f_l(k)$ is analytic in a neighborhood of $k=0$, then the statement is simply that, if $f_l(0)=0$, then the zero is simple for $l=0$ and double for $l \geq 1$.

We may now draw a conclusion concerning the number of zeros of $f_l(k)$ in the lower half of the complex plane. The function $f_l(k)$ being regular analytic there, its zeros cannot have a point of accumulation except possibly at $k=0$ or $k=\infty$. These two points cannot be accumulation points of roots either, the former because of (4.25) and the latter because of (4.16). Consequently the number of zeros must be finite. This proves that the number of discrete eigenvalues (i.e., bound states) for a given l value must be finite if the potential satisfies (3.1). An absolute bound on the number n_l of bound states of angular momentum l was given by Bargmann[22]:

$$n_l < \int_0^\infty dr r |V(r)| / (2l+1), \tag{4.26}$$

which shows at the same time that the *total* number of bound states is finite.

In general we cannot say anything about the zeros of $f_l(k)$ in the upper half of the complex plane. They do not indicate eigenvalues. If $f_l(k_0)=0$ and both k_0 and $-k_0^*$ are in a region of analyticity of $f_l(k)$ connected with the real axis, then (4.7') shows that we must also have $f_l(-k_0^*)=0$. The roots then appear in pairs symmetric with respect to the imaginary axis. Furthermore, Eq. (4.1) shows that if $k_0^2 = -\kappa^2$, $\kappa > 0$, is a discrete eigenvalue so that $f_l(-i\kappa)=0$, and if $+i\kappa$ lies in a region of analyticity of $f_l(k,r)$ connected with the real axis then we cannot have $f_l(i\kappa)=0$. Particularly, if the potential satisfies (3.14), then $f_l(i\kappa)$ cannot vanish if $-\kappa^2$ is an eigenvalue with $\kappa < a$. In other words, $f_l(i\kappa)$ can vanish under these circumstances only at the expense of a singularity of $f_l(k,r)$ at $k=i\kappa$.

If the potential vanishes identically beyond a finite distance R then quite a bit can be said about the zeros of $f_l(k)$. First of all, $f_l(k)$ must then have infinitely many complex roots in the upper half-plane. That fact is shown as follows.[23] The function

$$g_l(k^2) \equiv f_l(k) f_l(-k) \tag{4.27}$$

is in that case an entire function of k^2. Because of (2.22), (3.13), and (4.4) the asymptotic behavior of $f_l(k)$ when $\mathrm{Im}k \to +\infty$ is

$$f_l(k) \sim -(-)^l (2ik)^{-1} e^{-2ikR} \int_0^R dr V(r) e^{-2ik(r-R)}, \tag{4.28}$$

and hence by (4.16) that of $g_l(k^2)$ is the same. Suppose then that near $r=R$ the potential has an asymptotic expansion whose first term is

$$V(r) \sim c(R-r)^\sigma, \quad \sigma \geq 0. \tag{4.29}$$

Then (4.28) and (4.16) imply that as $\mathrm{Im}k \to +\infty$

$$g_l(k^2) \sim \text{const.} \times k^{-\sigma-2} e^{-2ikR}. \tag{4.28'}$$

Therefore, the *order*[27] of $g_l(k^2)$ is $\frac{1}{2}$. But an entire function of nonintegral order has necessarily an infinite number of zeros.[29] Because of (4.28'), moreover, and

[22] V. Bargmann, Proc. Natl. Acad. Sci. U. S. 38, 961 (1952).

[23] This was shown first by Humblet,[24] then independently by Rollnik.[25] The more general proof below follows Regge.[26]

[24] J. Humblet, Mém. Soc. roy. sci. Liège, 4, 12 (1952).

[25] H. Rollnik, Z. Physik 145, 639 and 654 (1956).

[26] T. Regge, Nuovo Cimento 8, 671 (1958).

[27] The definition of the order ρ of an entire function is

$$\rho \equiv \limsup_{r\to\infty} (\log \log M(r) / \log r),$$

where $M(r)$ is the maximum modulus of the function for $|z|=r$, see Boas,[28] p. 8.

[28] R. P. Boas, *Entire Functions* (Academic Press, Inc., New York, 1954).

[29] See Boas,[28] p. 24.

the analyticity of g_l, only a finite number of them can lie on the imaginary axis. As a result, $g_l(k^2)$ has infinitely many *complex* roots, which appear symmetrically with respect to the real axis and with respect to the imaginary axis. Those in the upper half-plane must be roots of $f_l(k)$ and those in the lower, of $f_l(-k)$.

The same argument which excludes infinitely many zeros on the imaginary axis also excludes infinitely many zeros above any ray through the origin, since there also the right-hand side of (4.28′) has no zeros. At the same time it follows from (4.15) that $f_l(k) \to 1$ as $|k| \to \infty$ on any line parallel to the real axis in the upper half plane; consequently, the number of zeros in any strip above the real axis is finite. In other words, although the total number of roots is infinite, for any given positive numbers μ and ν there is but a finite number of them with imaginary part less than ν or with a ratio of imaginary to real part greater than μ.

Since it follows from (4.16) that

$$\int_1^\infty dk k^{-2} \log g_l(k^2) < \infty,$$

we can also immediately draw the conclusion that if $\{k_n\}$ are the roots of $f_l(k)$, then[30]

$$\sum_n |\mathrm{Im}(k_n^{-1})| < \infty.$$

Since the roots of $f_l(k)$ appear in pairs symmetric with respect to the imaginary axis we can also say that

$$\sum k_n^{-1} \text{ converges}$$

provided that we always add k_n^{-1} and $(-k_n^*)^{-1}$ together first.

The distribution of zeros k_n in the right half-plane can be shown[31] in more detail to be such that as $n \to \infty$

$$\begin{aligned} \mathrm{Re}k_n &= n\pi/R + O(1), \\ \mathrm{Im}k_n &= [(\sigma+2)/2R] \log n + O(1). \end{aligned} \tag{4.30}$$

The entire function $f_l(k)$ can now be written in the form of an infinite product. (We are still dealing with the case in which $V=0$ for $r>R$.) According to Hadamard's factorization theorem[32] we can write

$$f_l(k) = f_l(0) e^{-ick} \prod_1^\infty \left(1 - \frac{k}{k_n}\right) e^{k/k_n} \tag{4.31}$$

assuming for simplicity $f_l(0) \neq 0$.[33] The constant c can be evaluated by means of a theorem by Pfluger[34] which tells us that the asymptotic behavior for large $|k|$ of (4.31) is for $k = \pm i|k|$

$$|k|^{-1} \log |f_l(k)/f_l(0)| = A \mp \sum \mathrm{Im}k_n^{-1} \pm c + o(1).$$

Comparison with (4.16) and (4.28′) shows that the right-hand side must equal $2R$ for $k = i|k|$, and zero, for $k = -i|k|$; hence, we must have

$$c + i \sum k_n^{-1} = R,$$

and consequently[26]

$$f_l(k) = f_l(0) e^{-ikR} \prod_1^\infty (1 - k/k_n). \tag{4.31′}$$

If we differentiate the logarithm of this equation and set $k=0$ we obtain at once by (4.9)

$$R + \frac{d}{dk}\delta_l(k)\bigg|_{k=0} = \sum \mathrm{Im}k_n/|k_n|^2. \tag{4.32}$$

The only negative contributions on the right-hand side come from the bound states.

It should be reemphasized that all of the foregoing detailed conclusions are true only if the potential vanishes identically beyond a finite point.

We may now compare φ_l to the physical wave function ψ_l. Equation (4.8) shows the difference in their analytic properties. Under the hypotheses (3.1) $\psi_l(k,r)$ is in general regular only in the upper half of the complex k plane. But even there it has simple poles at $k = i|k_0|$ if k_0^2 is an eigenvalue. That is the reason why, in contrast to $\varphi_l(k,r)$, the physical wave function $\psi_l(k,r)$ cannot always be expanded in a Born series.

If we think of the potential multiplied by a possibly complex scale factor λ,

$$V \to \lambda V, \tag{4.33}$$

then we saw that $\varphi_l(k,r)$ can always be expanded in a power series in λ which converges absolutely for all values of λ, and so can $f_l(k)$. If, however, for a given value of k, $f_l(-k)=0$ when λ has some complex value λ_0, then the power series in λ for $\psi_l(k,r)$ (Born series) will certainly not converge absolutely for $\lambda \geq \lambda_0$. Thus the Born series for ψ_l will have a finite radius of convergence.

The inequality (4.15) shows directly an important fact about the Born series. Since for every λ, $f_l(k)$ differs arbitrarily little from unity when k is made large enough (real or in the lower half plane) $f_l(k)$ can, for any given complex λ, have no zeros on the real axis beyond a certain point. Hence for every potential that satisfies (3.1), the Born series for $\psi_l(k,r)$ will necessarily converge absolutely if only k is large enough. Furthermore, if k is sufficiently large, the first Born approximation is good.

As a function of E, ψ_l has a branch cut along the positive real axis. On the "physical" sheet ($\mathrm{Im}k \geq 0$) of its Riemann surface ψ_l is a regular analytic function of E, except for simple poles at the bound state energies $E = -|E_n|$. At $E=0$ it is at worst $O(E^{\frac{1}{2}})$ (when approached inside the first sheet of the Riemann surface).

[30] See Boas,[28] p. 134; the argument is due to Regge.[26]

[31] See Humblet,[24] p. 45; also Regge,[26] which contains an error of a factor of π in the denominator of Eq. (19).

[32] See, for example, Boas,[28] p. 22.

[33] Otherwise we must replace $f_l(0)$ by const$\times k$ for $l=0$, or by const$\times k^2$ for $l \geq 1$.

[34] A. Pfluger, Comm. Math. Helv. **16**, 1 (1943); theorem 6B.

5. PROPERTIES OF THE S MATRIX

We may now use (4.5) in order to draw conclusions concerning the S matrix from the properties of $f_l(k)$.

On the real axis S_l is continuous and because of (4.16)

$$\lim_{k\to\pm\infty} S_l(k)=1. \tag{5.1}$$

For any potential that satisfies (3.1) the phaseshift thus necessarily approaches an integral multiple of π at high energies. If, in addition, the potential is integrable at $r=0$ then (4.16′) yields immediately the Born approximation result as $k\to\pm\infty$

$$k\tan\delta_l(k)=-\frac{1}{2}\int_0^\infty drV(r)+o(1). \tag{5.1′}$$

If all we know about the potential is (3.1) then we can say nothing about the properties of $S_l(k)$ in the complex plane, since as soon as we leave the real axis either $f_l(k)$ or $f_l(-k)$ may fail to be regular. In other words, $S_l(k)$ may have singularities of any type anywhere in the complex plane off the real axis. We cannot even conclude from (4.5) that $S_l(k)$ has a pole at $k=i|k_0|$ is k_0^2 is a discrete eigenvalue, because $f_l(i|k_0|)$ may be zero.

If, however, the potential satisfies (3.14) then $S_l(k)$ is necessarily an analytic function regular in the strip $0\leq \mathrm{Im}k<a$, except for simple poles at $k=i\kappa_n$ whenever $-\kappa_n^2$ is an eigenvalue and $0<\kappa_n<a$. In specific cases the analytic continuation of $S_l(k)$ may be carried further than $|\mathrm{Im}k|=a$ by the argument following (4.7′); namely, the continuation of successive terms in the Born approximation.

If the potential decreases asymptotically more rapidly than every exponential, particularly if it vanishes identically outside a finite region, then S_l is regular in the entire upper half-plane except for simple poles at $k=i\kappa_n$, $\kappa_n>0$, whenever $-\kappa_n^2$ is a discrete eigenvalue. The residues at such poles are readily found[35] by (4.20), (4.21′), and (4.8):

$$\begin{aligned}\mathrm{Res}_n&=1/\dot{S}_l(-i\kappa_n)\\&=\frac{(-)^{l+1}i[f_l(i\kappa_n)]^2}{4\kappa_n^{2l+2}\int_0^\infty dr[\varphi_l(-i\kappa_n,r)]^2}\\&=i\Big/4\int_0^\infty dr[\psi_l(-i\kappa_n,r)]^2,\end{aligned} \tag{5.2}$$

which is purely imaginary and

$$-i(-)^l\,\mathrm{Res}_n>0.$$

In the lower half of the complex plane singularities may again occur anywhere. If the potential fulfills (3.14) then $S_l(k)$ is regular there for $-\mathrm{Im}k<a$, except at isolated points where it may have poles of finite order. The latter occur at the zeros of $f_l(-k)$. For a potential of finite range that statement holds for the entire lower half-plane.

For a potential of type (3.14) then the zeros of $f_l(k)$ in the upper half-plane sufficiently close to the real axis lead to resonancelike peaks in $S_l(k)$ on the real axis.[38] The zeros of $f_l(k)$ on the positive imaginary axis are sometimes referred to as "virtual bound states." For a potential of finite range R we may immediately refer to the detailed discussion in Sec. 4 of the distribution of zeros of $f_l(k)$ in the upper half-plane. Thus there is always at most a finite number of virtual states and an infinite number of "resonances" distributed as shown in (4.30).

It is worthwhile to translate some of the foregoing statements into the language of *energy*. $S_l(E)$ then has a branch line along the positive real axis. If the potential satisfies (3.14) then $S_l(E)$ is an analytic function on a two sheeted Riemann surface, regular on the "physical sheet" ($\mathrm{Im}k\geq 0$) for $|E|<\hbar^2a^2/2\mu$, except for simple poles at $E=-|E_n|$, where E_n are the energies of bound states; on the sheet reached via the cut along the positive real axis $S_l(E)$ is regular for $|E|<\hbar^2a^2/2\mu$, except at a number of discrete points where it may have poles of finite order. The latter, if sufficiently close to the positive real axis, lead to resonancelike peaks in the functional behavior of $S_l(E)$ for positive E.

If the potential vanishes identically for $r>R$ then the foregoing statements hold on the entire Riemann surface (except at infinity); furthermore, on the first sheet we then have by (4.16) and (4.17)

$$\lim_{|E|\to\infty}[S_l(E)-1]e^{2ikR}=0. \tag{5.3}$$

If in addition the potential is absolutely integrable at the origin, then

$$[S_l(E)-1]|k|e^{2ikR}=O(1)\quad\text{as}\quad|E|\to\infty. \tag{5.3′}$$

In either case one may apply Cauchy's theorem to the integral

$$\int\frac{dE'[S_l(E')-1]e^{2ik'R}}{E'-E}$$

over a contour running above and below the branch cut and closed by a circle of large radius on the first sheet of the Riemann surface. Since the values of S_l on the upper and lower rim of the cut are related according to (4.5)–(4.7) by

$$S_l(E+i\epsilon)=S_l^*(E-i\epsilon),$$

[35] This result was first written down explicitly for $l=0$ by Lüders[36]; see also Hu.[37]

[36] G. Lüders, Z. Naturforsch. **10a**, 581 (1955).

[37] N. Hu, Phys. Rev. **74**, 131 (1948).

[38] I should prefer not to refer to these peaks as resonances but to reserve that name for peaks which are indeed caused by a physical resonance phenomenon. Otherwise the term loses its physical content. In that sense, then, a single channel problem never has resonances except for the low energy type associated with a bound or "almost bound" virtual state. For the same reason I should not like to refer to the complex zeros of $f_l(k)$ as decaying or radioactive states.

the result is the dispersion relation,[39]

$$\mathrm{Re}[(S_l(E)-1)e^{2ikR}]=\sum_n \frac{(E_n/\kappa_n)\,\mathrm{Res}_n \exp(-2\kappa_n R)}{E-E_n} + \frac{1}{\pi}P\int_0^\infty dE' \frac{\mathrm{Im}[(S_l(E')-1)e^{2ik'R}]}{E'-E}, \quad (5.4)$$

where $E_n=-\hbar^2\kappa_n^2/2\mu$ are the bound state energies, $\{\mathrm{Res}_n\}$ are the residues of S_l at $k=i\kappa_n$ given by (5.2), and P denotes the Cauchy principal value. Because of the presence of e^{2ikR} this is not a very useful equation.

More practically, we may represent the S matrix by the use of (4.31′) as an infinite product[40]:

$$S_l(k)=e^{-2ikR}\prod_{n=1}^{\infty}\frac{k_n-k}{k_n+k}. \quad (5.5)$$

This amounts to writing the phase shift as

$$\delta_l(k)=-kR-\sum_{n=1}^{N}\tan^{-1}\frac{k}{\kappa_n} + \sum_{n=1}^{N'}\tan^{-1}\frac{k}{\kappa_n'}+\sum_{\alpha=1}^{\infty}\tan^{-1}\frac{2kk_\alpha^{(2)}}{|k_\alpha|^2-k^2}, \quad (5.5')$$

where $E_n=-\hbar^2\kappa_n^2/2\mu$ are the bound state energies, $E_n'=-\hbar^2\kappa_n'^2/2\mu$ are the virtual state energies, and $E_\alpha=\hbar^2(k_\alpha^{(1)}+ik_\alpha^{(2)})^2/2\mu$, with $k_\alpha^{(1)}>0$, $k_\alpha^{(2)}>0$, are the "resonances." The distribution of the energies E_α is such that for any two given positive numbers c and d there exists only a finite number of E_α's above the ray $\mathrm{Im}E_\alpha=c\,\mathrm{Re}E_\alpha$ or below the parabola $\mathrm{Im}E_\alpha=2d\times(d^2+\mathrm{Re}E_\alpha)^{\frac{1}{2}}$.

Notice that each term in the α-sum contributes an increase in the phaseshift by π in the vicinity of $k\approx|k_\alpha|$. The contribution of the linear decrease in the first term, however, is such that almost all these increases are compensated by subsequent decreases. If the rising part of the curve leads to a "resonance" (i.e., a value of δ_l which is an odd multiple of $\frac{1}{2}\pi$) then so must the falling part (for almost all α), although that type of "resonance" bears no relation to the k_α.

Another point to notice is that, in spite of the appearance of infinitely many "resonance" terms in (5.5′), because of (5.1) only a finite number of them can actually lead to $\sin^2\delta_l=1$. There always exists an energy beyond which this can no longer occur.[41] Furthermore, it is easily seen by means of (4.30) that the maximal slope of individual terms in the α sum, which for large α occurs at $k\sim k_\alpha{}^{(1)}$, tends to naught as $1/k_\alpha{}^{(2)}$. Consequently, not only are there but a finite number of "resonance" points, but beyond a certain energy the phase shift becomes monotonely decreasing.

Another way of representing $S_l(k)$ if $V(r)=0$ for $r>R$ is a Mittag-Leffler expansion.[42] In order to do that we need an estimate for the residues of $S_l(k)$ at $k=-k_n$ if $f_l(k_n)=0$. Because of the distribution of zeros given by (4.30) and by (4.4) the leading terms of $f_l(k)$ in the vicinity of k_n when $n\to\infty$ are [assuming integrability of $V(r)$]

$$f_l(k)=1-(-)^l(2ik)^{-1}\int_0^R drV(r)e^{-2ikr}+O(k_n^{-1}), \quad (5.6)$$

while

$$\dot{f}_l(k)=(-)^l k^{-1}\int_0^\infty drrV(r)e^{-2ikr}+O(k_n^{-1}).$$

If we assume (4.29) then it is readily seen that we get

$$\dot{f}_l(k)=-2iR[f_l(k)-1]+O(k_n^{-1})$$

since for large k only the vicinity of $r=R$ contributes to the integral. If we now evaluate $\dot{f}_l$ at $k=k_n$ then we obtain,

$$\dot{f}_l(k_n)=2iR+O(k_n^{-1}). \quad (5.7)$$

Consequently, the residue of $S_l(k)$ at $k=-k_n$,

$$R_n=-f_l(-k_n)/\dot{f}_l(k_n)$$

is by (4.16′),

$$R_n=i/2R+O(k_n^{-1}). \quad (5.8)$$

As a result of (5.8), (4.6) and its unitarity, the S matrix can be written[24]

$$S_l(k)=1+kP_l(k)-k\sum_n\left(\frac{R_n/k_n}{k+k_n}+\frac{R_n^*/k_n^*}{k-k_n^*}\right), \quad (5.9)$$

where $P_l(k)$ is an entire function of k and it is understood that $\mathrm{Re}k_n\geq 0$, and that for the finite number of purely imaginary poles of $S_l(k)$, R_n is *one-half* the (purely imaginary) residue. Since by (5.8) and (4.30) for large n

$$\frac{R_n}{k_n^2}+\frac{R_n^*}{k_n^{*2}}=iR(\pi n)^{-2}+O(n^{-4}\log^2 n),$$

the series in (5.9) converges for all k and the Mittag-Leffler expansion is established.

As a consequence of (5.9) we can write

$$\mathrm{Re}[1-S_l(k)]=2\sin^2\delta_l(k) = EQ_l(E)+E\sum_n\frac{A_n(E-E_n)+\frac{1}{2}B_n\Gamma_n}{(E-E_n)^2+\frac{1}{4}\Gamma_n^2}, \quad (5.9')$$

[39] See, e.g., E. Corinaldesi, Nuclear Phys. **2**, 420 (1956).

[40] Such a product representation was written down by Hu,[37] for example, but not proved. It was proved under the conditions of this paper by Regge.[26]

[41] It is easily seen by considering $h_l(k)\equiv f_l(k)+f_l(-k)$ that whenever the potential is at least exponentially decreasing at infinity there can be only a finite number of points where $\sin^2\delta_l=1$, i.e., $h_l(k)=0$. In that case $h_l(k)$ is analytic on the real axis and, by (4.16), approaches unity at $k\to\pm\infty$; hence it cannot have infinitely many real zeros. If the potential does not satisfy (3.14) for any positive value of a then no such conclusion can be drawn.

[42] See, for instance, C. Caratheodory, *Functionentheory I* (Birkhäuser, Basel, 1950), p. 215 ff. This was first proved by Humblet[24] although written down without proof before, for example, by Hu.[37] The argument below is a simplified and somewhat less rigorous version of Humblet.[24]

where

$$A_n+iB_n=2R_n/k_n,$$
$$E_n+\tfrac{1}{2}i\Gamma_n=\hbar^2k_n^2/2\mu,$$

and

$$Q_l(E)=\tfrac{1}{2}[P_l(-k)-P_l(k)]k/E$$

is an entire function of E. The residues R_n can be expressed in terms of the k_n. By (5.5) we have

$$\frac{R_n}{k_n}=2e^{2ik_nR}\prod_{m\neq n}\frac{k_m+k_n}{k_m-k_n}. \tag{5.10}$$

The entire function $P_l(k)$ is also determined by the k_n; but no simple expression is known.

An interesting relation between the phase shift and the wave function, when the potential vanishes for $r>R$, is obtained as follows:

Differentiating the equivalent of (4.19) for $f_l(k,r)$ and $\varphi_l(k',r)$ with respect to k' and then setting $k=k'$ yields after integration

$$W[f_l(k,r),\dot{\varphi}_l(k,r)]=-2k\int_0^r dr' f_l(k,r')\varphi_l(k,r')$$

since $\dot{\varphi}_l'(k,r)=o(r^l)$ and $\dot{\varphi}_l(k,r)=o(r^{l+1})$ as $r\to 0$. Differentiation of (4.3) with respect to k therefore yields

$$\dot{f}_l(k)=lk^{-1}f_l(k)-2k^{l+1}\int_0^r dr' f_l(k,r')\varphi_l(k,r')+k^lW[\dot{f}_l(k,r),\varphi_l(k,r)],$$

where $r\geq R$. We then find by (4.1) that

$$\frac{\dot{f}_l(k)}{f_l(k)}-\frac{\dot{f}_l(-k)}{f_l(-k)}=\frac{d}{dk}\log S_l(k)$$
$$=\frac{2ik^{2l}}{|f_l(k)|^2}\Big\{2k^2\int_0^r dr'\varphi_l^2(k,r')-r[\varphi_l'^2(k,r)-\varphi_l(k,r)\varphi_l''(k,r)]+\varphi_l(k,r)\varphi_l'(k,r)\Big\},$$

or by (4.8), for $r\geq R$,

$$\frac{d}{dk}\delta_l(k)=2\int_0^r dr'|\psi_l(k,r')|^2-k^{-2}\{r[|\psi_l'(k,r)|^2-\psi_l''(k,r)\psi_l^*(k,r)]-\psi_l'(k,r)\psi_l^*(k,r)\}. \tag{5.11}$$

This equation takes on its most transparent form for $l=0$. Since it follows from (5.11) that

$$2|\psi_l(k,r)|^2=k^{-2}\frac{d}{dr}\{\ \},$$

we may also write

$$\frac{d}{dk}\delta_0(k)=2\int_0^\infty dr[|\psi_0(k,r)|^2-|\psi_0^{\text{out}}(k,r)|^2]+\tfrac{1}{2}k^{-1}\sin 2\delta_0(k), \tag{5.11'}$$

where ψ_l^{out} is the free wave function equal to ψ_l for $r\geq R$ and then continued in for $r<R$. For $l\neq 0$ this cannot be done since ψ_l^{out} is then not square integrable at the origin. Equation (5.11') directly illuminates the significance of a "resonance." Whenever the phaseshift varies rapidly upwards it means that there is a large probability for the particles to be found inside the region of interaction.

We may also write ψ_0^{out} explicitly; thus[43]

$$\frac{d}{dk}\delta_0(k)=2\int_0^R dr|\psi_0(k,r)|^2-R+\tfrac{1}{2}k^{-1}\sin(2kr+2\delta_0). \tag{5.11''}$$

It follows from this that

$$(d/dk)\delta_0(k)>-R+\tfrac{1}{2}k^{-1}\sin(2kr+2\delta_0)\geq-(R+\tfrac{1}{2}k^{-1}). \tag{5.12}$$

We may also compare Eq. (5.11) with (5.5); that leads to

$$2\int_0^\infty dr[|\psi_0(k,r)|^2-|\psi_0^{\text{out}}(k,r)|^2]+\tfrac{1}{2}k^{-1}\sin 2\delta_0(k)=\sum_n\frac{ik_n}{k_n^2-k^2}-R. \tag{5.13}$$

It should be recalled at this point that all the results from Eq. (5.3) on assumed that the potential vanishes identically for $r>R$. We now return to the general case, assuming only (3.1).

The low-energy behavior of $S_l(k)$ is established as follows: The analytic function $f_l(k)$ being regular in the lower half of the complex k plane, we have

$$\frac{1}{2\pi i}\int_C d\log f_l(k)=n_l, \tag{5.14}$$

where n_l is the number of zeros of $f_l(k)$ in the lower half-plane and the path of integration C runs along the real axis from $+\infty$ to $-\infty$, avoiding the origin by a small semicircle of radius ϵ in the lower half-plane, and closed by a large semicircle of radius K in the lower half-plane. Since each discrete eigenvalue produces a simple zero of $f_l(k)$, n_l is the number of bound states of angular momentum l.

The contribution to (5.14) from the large semicircle vanishes by (4.16) in the limit as $K\to\infty$. If near $k=0$ we write[44]

$$f_l(k)=ak^q+o(k^q)$$

[43] This equation and the following inequality were given by Lüders.[36] The inequality (5.12) and the corresponding one obtainable from (5.11) for $l=1$ were first derived by Wigner under more general assumptions; E. P. Wigner, Phys. Rev. **98**, 145 (1955).

[44] It is sufficient that that is true in every cone of opening less than π in the lower half-plane.

then the contribution from the small semicircle is

$$\int_{\supset} d\log f_l(k) \to q\int_{\supset} d\log k = -i\pi q$$

in the limit as $\epsilon \to 0$. Consequently, (5.14) becomes, by (4.9),

$$\lim_{\epsilon\to 0}\lim_{K\to\infty}\left[\delta_l(-K)-\delta_l(-\epsilon)+\delta_l(\epsilon)-\delta_l(K) + i\log\left|\frac{f_l(K)}{f_l(-K)}\cdot\frac{f_l(-\epsilon)}{f_l(\epsilon)}\right|\right] = 2\pi(n_l+\tfrac{1}{2}q).$$

The imaginary term vanishes by (4.7). Furthermore, because of (4.7), $\delta_l(k)$ may be defined to be an odd function of k. We have therefore

$$\delta_l(0)-\delta_l(\infty) = \pi(n_l+\tfrac{1}{2}q).$$

A glance at (4.25) and (4.25′) shows that $q=0$ if $f_l(0)\neq 0$; $q=1$ if $f_l(0)=0$ and $l=0$; $q=2$ if $f_l(0)=0$ and $l\geq 1$. In the last case, as we saw, $k=0$ is a discrete eigenvalue and should thus be added to n_l. As a result we obtain the Levinson theorem[45]

$$\delta_l(0)-\delta_l(\infty) = \begin{cases}\pi(n_l+\frac{1}{2}), & \text{if } l=0 \text{ and } f_l(0)=0,\\ \pi n_l, & \text{otherwise,}\end{cases} \tag{5.15}$$

which constitutes the only generally valid relation between scattering phaseshifts and bound states.

Because of (4.16), $\delta_l(\infty)$ may always be defined to be zero. Equation (5.15) then determines the value of the phaseshift at zero energy. As a consequence of (5.15) we have

$$S_l(0) = \begin{cases}-1, & \text{if } l=0 \text{ and } f_l(0)=0,\\ 1, & \text{otherwise.}\end{cases} \tag{5.16}$$

Notice that $S_l(0)=-1$ implies by (2.15) that the scattering amplitude becomes infinite at $E=0$. This happens whenever the potential is such that the slightest strengthening will introduce a new bound state of zero angular momentum. This is usually referred to as a zero-energy resonance.

The next question that arises is how $S_l(k)$ approaches its limiting value at $k=0$. The answer is given most simply by using (2.21) in combination with (4.8)

$$S_l(k) = 1-2ik^l\int_0^\infty dr u_l(kr)V(r)\varphi_l(k,r)/f_l(-k). \tag{5.17}$$

[45] Although this theorem was known before in less precise form, it was proved first by Levinson.[13] The proof given here follows Levinson. It has been proved under more general hypotheses, namely, only the completeness of the set of eigenfunctions by J. Jauch, Helv. Phys. Acta **30**, 143 (1957); see also A. Martin, Nuovo cimento **7**, 607 (1958).

The inequalities (3.9) and (3.11) show that

$$|S_l(k)-1| \leqslant C|k|^{2l+1}\int_0^\infty dr|V(r)| \times\left(\frac{r}{1+|k|r}\right)^{2l+2}\Big/|f_l(k)|. \tag{5.18}$$

If $f_l(0)\neq 0$ then we may conclude that the right-hand side is $O(k^{2l+1})$ *provided* that[46]

$$\int_0^\infty dr|V(r)|r^{2l+2} < \infty.$$

If $f_l(0)=0$, then it follows from (4.25) that the right-hand side of (5.18) is $O(k^{2l-1})$ for $l\geq 1$, and $O(1)$ for $l=0$. Consequently, if the potential satisfies the foregoing restriction, then as $k\to 0$,

$$S_l(k)-1 = 2ie^{i\delta_l}\sin\delta_l = \begin{cases}-2, & \text{if } l=0 \text{ and } f_l(0)=0,\\ O(k^{2l+1}), & \text{otherwise.}\end{cases} \tag{5.19}$$

If there is a bound state of zero energy (which is possible only if $l\geq 1$), then as $k\to 0$

$$S_l(k)-1 = O(k^{2l-1}). \tag{5.19′}$$

We may generate a Born series for $S_l(k)$ by using (5.17). Just as in the case of $\psi_l(k,r)$, it is the presence of $f_l(-k)$ in the denominator which may prevent the convergence; as (5.18) shows, the numerator converges absolutely. We may, therefore, draw the same conclusion as at the end of Sec. 4. For every potential that fulfills (3.1) there exists an energy beyond which the S matrix can be expanded in an absolutely convergent Born series. Furthermore, it follows from (5.17) together with (4.16) and (3.13) that in the high-energy limit the first term in the Born series is a good approximation.

Suppose that the potential $V=-|U|$ produces neither a bound state of $l=0$ nor a "zero energy resonance." Then $f_0(0)\neq 0$; the replacement (4.33) with $|\lambda|\leq 1$ cannot make $f_0(0)=0$ either, for that would imply

$$-\lambda\int_0^\infty drV(r)|\varphi_0(0,r)|^2 = -\int_0^\infty dr\varphi_0^*(0,r)\varphi_0''(0,r) = \int_0^\infty dr|\varphi_0'(0,r)|^2,$$

which is possible only for real λ. As a result the Born series for

$$\lim_{k\to 0}[S_0(k)-1]/k = \dot{f}_0(0)/f_0(0)$$

[46] D. S. Carter, Ph.D. thesis, Princeton University, 1952 (unpublished).

converges absolutely. A glance at (2.15) shows that because of (5.19) the Born series for the scattering amplitude at zero energy then converges absolutely. But insertion of (2.2) and of the middle form of (2.3) in (2.12) shows that the Born series for $\Theta(\mathbf{k}',\mathbf{k})$ using U is dominated by that for $\Theta(0,0)$ using $V=-|U|$. Consequently, a sufficient criterion for the Born series for the scattering amplitude of a potential U to converge absolutely at all energies is that $V=-|U|$ produce no s wave bound states or zero energy resonance.[47]

We finally want to look at a question of more restricted applicability: Is it possible to determine the Jost function $f_l(k)$ from the knowledge of $S_l(k)$? The answer is "yes," provided that we know also *in addition* the energies of the bound states. [Their number is already determined by $S_l(k)$ according to (5.15).]

If there are n_l bound states with energies $-\hbar^2\kappa_n^2/2\mu$, $\kappa_n\geq 0$, then we know that $S_l(k)$ can be written by (4.5) as

$$S_l(k)=\prod_{n=1}^{n_l}\left(\frac{k+i\kappa_n}{k-i\kappa_n}\right)^2 S_l^{\mathrm{red}}(k),$$

where

$$S_l^{\mathrm{red}}(k)=f_l^{\mathrm{red}}(k)/f_l^{\mathrm{red}}(-k),$$

and

$$f_l^{\mathrm{red}}(k)=\prod\frac{k-i\kappa_n}{k+i\kappa_n}f_l(k) \tag{5.20}$$

is an analytic function regular in the lower half of the complex plane, without any zeros there, and with

$$f_l^{\mathrm{red}}(k)\underset{|k|\to\infty}{\longrightarrow}1$$

there. Therefore $\log f_l^{\mathrm{red}}(k)$ is analytic in the lower half-plane and vanishes at infinity; consequently, it satisfies a simple "dispersion relation." By Cauchy's theorem

$$\log f_l^{\mathrm{red}}(k)=-\frac{P}{\pi i}\int_{-\infty}^{\infty}dk'\frac{\log f_l^{\mathrm{red}}(k')}{k'-k},$$

and hence

$$\log|f_l(k)|=-\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{dk'\ \mathrm{Im}\log f_l^{\mathrm{red}}(k')}{k'-k}.$$

By (5.20) and (4.9) we have

$$\mathrm{Im}\log f_l^{\mathrm{red}}(k)=\delta_l(k)-2\textstyle\sum_n\cot^{-1}(k/\kappa_n)$$

and therefore[48]

$$\log|f_l(k)|=-\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{dk'\delta_l(k')}{k'-k}+\sum_n\log\frac{E-E_n}{E} \tag{5.21}$$

or

$$f_l(k)=\prod_n\left(1-\frac{E_n}{E}\right)\exp\left[-\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{dk'\delta_l(k')}{k'-k+i\epsilon}\right] \tag{5.21'}$$

in the limit as $\epsilon\to 0+$. This explicitly expresses $f_l(k)$ in terms of the phaseshift $\delta_l(k)$ (i.e., of $S_l(k)$) and the bound states.

6. GREEN'S FUNCTION

It is very easy now to write down a complete Green's function or resolvent of the radial Schrödinger equation (2.10). Such a function must satisfy the equation

$$\left[-\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)}{r^2}-k^2\right]\mathfrak{G}_l(k;r,r')=-\delta(r-r'). \tag{6.1}$$

It is therefore a solution of (2.10) for $r\neq r'$. At $r=r'$ its derivative suffers a discontinuity of unity:

$$\frac{d}{dr}\mathfrak{G}_l(k;r,r')\Big|_{r=r'-\epsilon}^{r=r'+\epsilon}=1. \tag{6.2}$$

Suppose, then, we want the Green's function appropriate to the boundary condition of (2.8), namely, such that it contains no incoming waves at infinity. It must then have the form

$$\mathfrak{G}_l(k;r,r')=\begin{cases}\varphi_l(k,r)a(k,r'), & r<r',\\ f_l(k,r)b(k,r'), & r>r'.\end{cases}$$

Since $\mathfrak{G}_l$ must be continuous at $r=r'$ we find that

$$a(k,r)=C(k)f_l(-k,r),$$
$$b(k,r)=C(k)\varphi_l(k,r).$$

The requirement (6.2) then fixes $C(k)$

$$C(k)W[\varphi_l(k,r),f_l(-k,r)]=1.$$

Because of (4.3) we then find that

$$C(k)=(-)^{l+1}k^l/f_l(-k).$$

As a result

$$\begin{aligned}\mathfrak{G}_l(k;r,r')&=(-)^{l+1}k^l\varphi_l(k,r_<)f_l(-k,r_>)/f_l(-k)\\&=(-)^{l+1}k^{-l}\psi_l(k,r_<)f_l(-k,r_>).\end{aligned} \tag{6.3}$$

From the analyticity of $\varphi_l(k,r)$, $f_l(k,r)$ and $f_l(k)$ we can therefore infer the following properties of the Green's function $\mathfrak{G}_l(k;r,r')$.

For each fixed r and r', $\mathfrak{G}_l(k;r,r')$ is an analytic function of k regular in the open upper half of the complex plane and continuous on the real axis, except for simple poles at $k=i\kappa_n$ if $-\kappa_n^2$ is a discrete eigenvalue, and except at $k=0$ where it may be as singular as $O(k^{-2})$ when approached from above the real axis (for $l=0$, it is at worst $O(k^{-1})$).

In the language of the energy E, $\mathfrak{G}_l(k;r,r')$ has a branch cut along the positive real axis. On the "physical" sheet of its Riemann surface ($\mathrm{Im}k\geq 0$) it is a regular analytic function except for a finite number of simple poles on the negative real axis at the position of the bound states. At $E=0$, it has a branch point and

[47] The foregoing argument is a slight generalization of that given by H. Davies, Nuclear Phys. 14, 465 (1960).

[48] The phaseshift is assumed to be defined so that it vanishes at infinity. A similar, but slightly less explicit form of $f_l(k)$ was given by Jost and Kohn.[49]

[49] R. Jost and W. Kohn, Phys. Rev. 87, 977 (1952).

may in exceptional cases be $O(E^{-1})$ when $E=0$ is approached from the first sheet of the Riemann surface. [For $l=0$, $O(E^{-\frac{1}{2}})$.] As $E\to\infty$ on the first sheet, it follows from (3.13), (3.17), and (3.16) that

$$\begin{aligned}\mathfrak{G}_l(E;r,r')&=G_l(E;r,r')+o(|k|^{-1}e^{-\nu|r-r'|})\\&=(2ik)^{-1}(e^{ik(r_>-r_<)}-(-)^l e^{ik(r_>+r_<)})\\&\quad+o(|k|^{-1}e^{-\nu|r-r'|}).\end{aligned}\tag{6.4}$$

The function $\mathfrak{G}_l(E;r,r')$ taken at the upper rim of its branch cut (i.e., at $k>0$) is usually denoted by $\mathfrak{G}_l^{(+)}$; when we follow its analytic continuation around the origin to the lower rim of the cut ($k<0$) we obtain $\mathfrak{G}_l^{(-)}$.

In general nothing can be said about a possible analytic continuation of $\mathfrak{G}_l$ beyond the branch cut onto the second sheet. If the potential satisfies (3.14), then it is regular there as far as $|E|<a^2\hbar^2/2\mu$, except possibly for poles of finite order. The latter, if sufficiently close to the positive real axis, lead to resonancelike peaks in the scattering amplitude. If the potential vanishes at infinity faster than every exponential (e.g., if it is identically zero beyond a finite point), then $\mathfrak{G}_l$ has an analytic continuation into the whole second sheet of its Riemann surface, where it then must have infinitely many poles of finite order.

The relation between $\mathfrak{G}_l$ and S_l is given directly by the solution of (2.8):

$$\psi_l(k,r)=u_l(kr)+\int_0^\infty dr'\mathfrak{G}_l(k;r,r')V(r')u_l(kr'),\tag{6.5}$$

which, inserted in (2.21), yields

$$\begin{aligned}S_l(k)=1-2ik^{-1}&\int_0^\infty dr u_l(kr)V(r)u_l(kr)\\&-2ik^{-1}\int_0^\infty dr\int_0^\infty dr' u_l(kr)V(r)\\&\times\mathfrak{G}_l(k;r,r')V(r')u_l(kr').\end{aligned}\tag{6.6}$$

The difference in analytic behavior between $S_l(k)$ and $\mathfrak{G}_l(k;r,r')$, the latter being regular in the upper half-plane (except for the bound state poles), while the former need not be regular there, comes from the possible divergence of the integrals in (6.6).

7. COMPLETENESS

We now want to prove the completeness of the set of eigenfunctions of the radial Schrödinger equation under the assumption (3.1) on the potential. The idea of the proof[50] is to evaluate the integral

$$\int dE\mathfrak{G}_l(E;r,r')$$

over a closed contour running along the two rims of the branch cut in the complex E plane and closed by a large circle at infinity on the first sheet of the Riemann surface. On the one hand, that integral is evaluated by Cauchy's residue theorem in terms of the bound state poles on the negative real axis. On the other hand, it is explicitly written down in terms of its various contributions. The whole procedure is a little simpler, however, in the k plane.

We consider the integral

$$I(r)\equiv\int_C kdk\int_0^\infty dr'h(r')\mathfrak{G}_l(-k;r,r'),\tag{7.1}$$

where $\mathfrak{G}_l$ is given by (6.3), $h(r)$ is an arbitrary sufficiently well behaved function of r (square integrability suffices), and the contour C of the k integration is the same as in (5.14).

The integral $I(r)$ is written

$$I=I_1+I_2$$

$$I_1(r)=-\int_C dkk^{l+1}\int_0^r dr'h(r')\varphi_l(k,r')f_l(k,r)/f_l(k)\tag{7.2}$$

$$I_2(r)=-\int_C dkk^{l+1}\int_r^\infty dr'h(r')f_l(k,r')\varphi_l(k,r)/f_l(k).\tag{7.3}$$

We first consider $I_1(r)$.

Suppose that the discrete eigenvalues are $-\kappa_n^2$. Then we write ($\kappa_n>0$)

$$\begin{aligned}\varphi_l^{(n)}(r)&\equiv\varphi_l(-i\kappa_n,r),\\f_l^{(n)}(r)&\equiv f_l(-i\kappa_n,r),\\C_n&\equiv\dot{f}_l(-i\kappa_n).\end{aligned}$$

Since $\varphi_l(k,r)$, $f_l(k,r)$, and $f_l(k)$ are analytic functions regular in the lower half of the complex plane and $f_l(k)$ has simple zeros at $k=-i\kappa_n$, the integral $I_1(r)$ is evaluated immediately by means of Cauchy's residue theorem

$$I_1(r)=-2\pi i\sum_n\int_0^r dr'h(r')\varphi_l^{(n)}(r')f_l^{(n)}(r)(-i\kappa_n)^{l+1}/C_n.$$

If we call

$$\int_0^\infty dr[\varphi_l^{(n)}(r)]^2\equiv N_n^2,$$

then (4.21′) reads

$$C_n=-2a_n(-i\kappa_n)^{l+1}N_n^2,$$

where

$$a_n=f_l^{(n)}(r)/\varphi_l^{(n)}(r).$$

Thus we obtain

$$I_1(r)=i\pi\sum_n\int_0^r dr'h(r')\varphi_l^{(n)}(r')\varphi_l^{(n)}(r)N_n^{-2}.\tag{7.4}$$

[50] This proof follows Jost and Kohn,[49] Appendix. It is the type of proof given by Titchmarsh, see E. C. Titchmarsh, *Eigenfunction Expansions I* (Oxford University Press, New York, 1946).

On the other hand, we evaluate I_1 directly. The contribution $I_{1\epsilon}$ to the k integral from the small semicircle vanishes in the limit as its radius tends to zero, except when $f_l(0)=0$. In that case it still vanishes for $l=0$, because of (4.25). For $l\geq 1$ we write

$$f_l(k)=c_0k^2+o(k^2).$$

The contribution from the small semicircle is then by (4.21) seen to be

$$I_{1\epsilon}(r)=-i\pi\int_0^r dr'h(r')\varphi_l^{(0)}(r')\varphi_l^{(0)}(r)N_0^{-2}, \quad (7.5)$$

where

$$\varphi_l^{(0)}(r)\equiv\varphi_l(0,r),$$

and

$$N_0^2\equiv\int_0^\infty dr[\varphi_l^{(0)}(r)]^2.$$

The contribution I_{1R} to I_1 from the large semicircle is evaluated by the use of the asymptotic functions for large $|k|$. Thus by (3.13) and (3.17)

$$I_{1R}\underset{R\to\infty}{\sim}\tfrac{1}{2}i\int_0^r dr'h(r')\int_{s.c.}dk(e^{-ik(r-r')}-(-)^le^{-ik(r+r')})$$

$$\underset{R\to\infty}{\sim}\tfrac{1}{2}h(r)\int_{s.c.}dkk^{-1}=\tfrac{1}{2}i\pi h(r). \quad (7.6)$$

The remaining contribution I_{1E} to I_1 is the integral over the real axis, where we may use the fact that $\varphi_l(k,r)$ is an even function of k and then (4.1) and (4.7); thus

$$I_{1E}(r)=\int_0^r dr'h(r')\left(\int_{-\infty}^{-\epsilon}+\int_{+\epsilon}^{\infty}\right)dkk^{l+1}$$
$$\times\varphi_l(k,r')f_l(k,r)/f_l(k)$$
$$=-i\int_0^r dr'h(r')\left(\int_{-\infty}^{-\epsilon}+\int_{+\epsilon}^{\infty}\right)dkk^{2l+2}$$
$$\times\varphi_l(k,r')\varphi_l(k,r)/|f_l(k)|^2.$$

We may now let $\epsilon\to 0$ and get

$$I_{1E}(r)=-2i\int_0^r dr'h(r')\int_0^\infty dkk^{2l+2}$$
$$\times\varphi_l(k,r')\varphi_l(k,r)/|f_l(k)|^2. \quad (7.7)$$

Equating the sum of (7.5)–(7.7) to (7.4) yields

$$h(r)=2\int_0^r dr'h(r')\left[2\int_0^\infty dkk^{2l+2}\frac{\varphi_l(k,r')\varphi_l(k,r)}{\pi|f_l(k)|^2}\right.$$
$$\left.+\sum_n\frac{\varphi_l^{(n)}(r')\varphi_l^{(n)}(r)}{N_n^2}\right], \quad (7.8)$$

where the sum now includes the bound state of zero binding energy if there is one.

We then go through the same arguments for $I_2(r)$, where we may replace the upper limit of the r' integration by $r+\mu$, μ being an arbitrary positive number. The result is

$$h(r)=2\int_r^{r+\mu}dr'h(r')\left[2\int_0^\infty dkk^{2l+2}\frac{\varphi_l(k,r')\varphi_l(k,r)}{\pi|f_l(k)|^2}\right.$$
$$\left.+\sum_n\frac{\varphi_l^{(n)}(r')\varphi_l^{(n)}(r)}{N_n^2}\right]. \quad (7.8')$$

We now add (7.8) and (7.8'), divide by two, and let $\mu\to\infty$. The ensuing improper integral will converge provided $h(r)$ is square integrable. The result can be written in the customary notation of a δ function

$$\frac{2}{\pi}\int_0^\infty dkk^{2l+2}\frac{\varphi_l(k,r)\varphi_l(k,r')}{|f_l(k)|^2}$$
$$+\sum_n\frac{\varphi_l^{(n)}(r)\varphi_l^{(n)}(r')}{N_n^2}=\delta(r-r'). \quad (7.9)$$

This proves the completeness of the set of wave functions of the continuous and discrete spectrum and shows at the same time what the necessary weight function is.

The weight function appearing in (7.9) is also defined as the *spectral function* $\rho_l(E)$ in the following sense. If we set

$$\frac{d\rho_l(E)}{dE}=\begin{cases}\dfrac{2\mu}{\pi\hbar^2}k^{2l+1}/|f_l(k)|^2, & E>0,\\ \sum_n\delta(E-E_n)/N_n^2, & E\leq 0,\end{cases} \quad (7.10)$$

with $\rho_l(-\infty)=0$, then (7.9) can be written as a Stieltjes integral

$$\int d\rho_l(E)\varphi_l(k,r)\varphi_l(k,r')=\delta(r-r'). \quad (7.9')$$

At the same time we may now write the resolvent (6.3)

$$\mathfrak{G}_l(E;r,r')=\frac{\hbar^2}{2\mu}\int d\rho_l(E')\frac{\varphi_l(k',r)\varphi_l(k',r')}{E-E'}. \quad (7.11)$$

On the upper rim of the branch cut we get the outgoing wave Green's function $\mathfrak{G}_l^{(+)}$; on the lower rim, the incoming wave Green's function $\mathfrak{G}_l^{(-)}$. The average of the two defines a real (standing wave) Green's function, $\mathfrak{G}_l^{(P)}$, for which the Cauchy principal value of the integral must be used.

A comparison of (7.9) with (4.8) shows that we may write the completeness in terms of the physical wave function ψ_l

$$\frac{2}{\pi}\int_0^\infty dk\psi_l(k,r)\psi_l^*(k,r')$$
$$+\sum_n\psi_l^{(n)}(r)\psi_l^{(n)}(r')=\delta(r-r'), \quad (7.9'')$$

where $\psi_l^{(n)}(r)$ are the bound-state wave functions normalized to unity

$$\psi_l^{(n)}(r)=\varphi_l(-i\kappa_n, r)/N_n.$$

The complete Green's function can similarly be written

$$\begin{aligned}&\mathfrak{G}_l(k; r,r')\\&=\frac{2}{\pi}\int_0^\infty dk'\frac{\psi_l(k',r)\psi_l^*(k',r')}{k^2-k'^2}+\sum_n\frac{\psi_l^{(n)}(r)\psi_l^{(n)}(r')}{k^2+\kappa_n^2}\\&=\frac{1}{\pi}\int_{-\infty}^\infty\frac{dk'}{k'}\frac{\psi_l(k',r)\psi_l^*(k',r')}{k-k'}+\sum_n\frac{\psi_l^{(n)}(r)\psi_l^{(n)}(r')}{k^2+\kappa_n^2},\end{aligned}\tag{7.11'}$$

where for real k the limit from above the real axis to positive k defines the outgoing wave Green's function, and to negative k, the incoming wave Green's function.

8. GEL'FAND-LEVITAN EQUATIONS

The equations first derived by Gel'fand and Levitan[51,52] have a special interest for the solution of the problem of going backwards, from a knowledge of the phaseshift and bound states to the underlying potential. However, they are useful sometimes also in other contexts.

Consider the function[53]

$$I(E,r)=\int d\rho_l^{(1)}(E')\varphi_l(k',r)\times\int_0^r dr'\varphi_l^{(1)}(k',r')\varphi_l^{(1)}(k,r'),\tag{8.1}$$

where the quantities with the superscript "1" refer to a given potential $V^{(1)}(r)$, and those without superscript, to another potential $V(r)$. If we insert (4.19) and (7.10) in (8.1) and use (4.1), we obtain

$$\begin{aligned}I=&\frac{i}{\pi}\int_{-\infty}^\infty\frac{dk'k'^{l+1}}{k^2-k'^2}\frac{\varphi_l(k',r)}{f_l^{(1)}(k')}W[\varphi_l^{(1)}(k,r),f_l^{(1)}(k',r)]\\&+\sum_n\frac{\varphi_l(-i\kappa_n,r)}{k^2+\kappa_n^2}\frac{1}{N_n^2}W[\varphi_l^{(1)}(k,r),\varphi_l^{(1)(n)}(r)],\end{aligned}\tag{8.2}$$

if κ_n refers to the bound states of $V^{(1)}(r)$ and we take k slightly off the real axis into the lower half-plane. Adding to the integral a similar one over a large semicircle in the lower half-plane, we can evaluate it by means of Cauchy's residue theorem. The result exactly cancels the bound state sum in (8.2). Thus we are left with the negative of the integral over the large semicircle where we may use the asymptotic functions for large k', given by (3.13), (3.17), and (4.16). The result is that

$$I(E,r)=\varphi_l(k,r)-\tfrac{1}{2}\varphi_l^{(1)}(k,r).\tag{8.3}$$

The next step is to notice that the completeness proof, i.e., the derivation of (7.8), would have gone through just as well if $\varphi_l(k,r')$ had been replaced by $\varphi_l^{(1)}(k,r')$. If in the resulting formula we set $h(r)=\varphi_l^{(1)}(k,r)$, we get

$$\tfrac{1}{2}\varphi_l^{(1)}(k,r)=\int d\rho_l(E')\varphi_l(k',r)\times\int_0^r dr'\varphi_l^{(1)}(k,r')\varphi_l^{(1)}(k',r').\tag{8.4}$$

The implication of (8.1), (8.3), and (8.4) is that

$$\varphi_l(k,r)=\varphi_l^{(1)}(k,r)+\int_0^r dr'K_l(r,r')\varphi_l^{(1)}(k,r'),\tag{8.5}$$

where

$$K_l(r,r')=\int d[\rho_l^{(1)}(E)-\rho_l(E)]\varphi_l(k,r)\varphi_l^{(1)}(k,r').\tag{8.6}$$

Equation (8.5) resembles that containing a complete Green's function; however, in contrast to the latter, $K_l(r,r')$ has the remarkable property of being independent of the energy. It obviously satisfies the differential equation

$$\begin{aligned}&\frac{\partial^2}{\partial r^2}K_l(r,r')-\left[V(r)+\frac{l(l+1)}{r^2}\right]K_l(r,r')\\&\quad=\frac{\partial^2}{\partial r'^2}K_l(r,r')-\left[V^{(1)}(r')+\frac{l(l+1)}{r'^2}\right]K_l(r,r').\end{aligned}\tag{8.7}$$

Inserting (8.5) in the Schrödinger equation and using (8.7) readily leads to

$$2\frac{d}{dr}K_l(r,r)=V(r)-V^{(1)}(r).\tag{8.8}$$

In addition, K_l satisfies the boundary condition

$$K_l(0,r)=0.\tag{8.9}$$

If we multiply, finally, (8.5) by $\varphi_l^{(1)}(k,r'')$ and integrate with the weight $\rho_l^{(1)}-\rho_l$, we obtain the Gel'fand Levitan integral equation

$$K_l(r,r')=g_l(r,r')+\int_0^r dr''K_l(r,r'')g_l(r'',r'),\tag{8.10}$$

where

$$g_l(r'',r')=\int d[\rho_l^{(1)}(E)-\rho_l(E)]\times\varphi_l^{(1)}(k,r'')\varphi_l^{(1)}(k,r').\tag{8.11}$$

[51] I. M. Gel'fand and B. M. Levitan, Doklady Akad. Nauk S.S.S.R. **77**, 557 (1951).
[52] I. M. Gel'fand and B. M. Levitan, Izvest. Akad. Nauk S.S.S.R. **15**, 309 (1951).
[53] The procedure follows Jost and Kohn.[54] See also N. Levinson, Phys. Rev. **89**, 755 (1953).
[54] R. Jost and W. Kohn, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **27**, No. 9 (1953).

It can be shown[54] that (8.10) always has a unique solution. A knowledge of the spectral function $\rho_l(E)$ thus determines $K_l(r,r')$ via (8.10) and (8.11); the function $\varphi_l(k,r)$ then follows from (8.5), and the potential, from (8.8). The spectral function in turn is given by (7.10) in terms of the bound state energies and the Jost function $f_l(k)$, and the latter is given by (5.21) in terms of the phase shift and the bound state energies. This demonstrates that in general, binding energies and scattering phaseshifts are completely independent, and that if there are n_l bound states, then there exists an n_l parameter (the N_n) family of potentials all of which lead to the same phaseshift and to the same binding energies.

A simple application is that in which the difference $\rho_l^{(1)}-\rho_l$ is infinitesimal, due to an infinitesimal change in the phaseshift.[55] In that instance one uses (5.21) and (7.11) in (8.6) and finds

$$K_l(r,r')=-\frac{2}{\pi}\int_{-\infty}^{\infty}dk'k'\delta\delta_l(k') \times\left[\mathfrak{G}_l^{(P)}(E';r,r')-\sum_n\frac{\psi_l^{(n)}(r)\psi_l^{(n)}(r')}{E'-E_n}\right]$$

to first order in the variation $\delta\delta_l(k)$ of the phaseshift. Consequently, by (8.8),

$$\frac{\delta V(r)}{\delta\delta_l(k)}=-\frac{4}{\pi}\frac{d}{dr}\left\{\mathfrak{G}_l^{(P)}(E;r,r)-\sum_n\frac{[\psi_l^{(n)}(r)]^2}{E-E_n}\right\}. \quad (8.12)$$

Specifically, for $r=0$, we have by (6.3), (3.3), and (4.3′)

$$\frac{d}{dr}\mathfrak{G}_l^{(P)}(E;r,r)\underset{r\to 0}{\longrightarrow}-\frac{1}{2l+1},$$

and therefore

$$\delta V(0)/\delta\delta_l(k)=4k/\pi(2l+1). \quad (8.13)$$

This equation can be integrated immediately

$$V(0)-V^{(1)}(0)=[8/\pi(2l+1)]\int_0^{\infty}dkk[\delta_l(k)-\delta_l^{(1)}(k)],$$

where $V(r)$ and $V^{(1)}$ must have the same bound states. Finally we use the Bargmann potentials (Sec. 10) in order to construct a potential $V^{(1)}$ with the same bound states as V and whose phaseshift is asymptotically equal to $\delta_l(k)$, i.e., the value given by (5.1′). The result is a simple exact relation between the value of the potential at the origin and the lth phaseshift and bound state energies $E_n^{(l)}(<0)$[55]:

$$V(0)=\frac{4}{2l+1}\left\{\frac{2}{\pi}\int_0^{\infty}dk\left[k\delta_l(k)+\frac{1}{2}\int_0^{\infty}drV(r)\right]-\sum_n E_n^{(l)}\right\}, \quad (8.14)$$

or

$$V(0)=\frac{4}{2l+1}\left\{-\frac{2}{\pi}\int_0^{\infty}dkk[\delta_l(k)+k\delta_l'(k)]-\sum_n E_n^{(l)}\right\}, \quad (8.14')$$

the prime indicating differentiation with respect to k. This shows that although the phaseshifts of the same potential are asymptotically equal for different l values and near $k=0$ become smaller as l increases, their first moments *increase* with growing l.

9. GENERALIZATION TO THE CASE WITH COUPLING

Almost everything done in the preceding sections can be generalized to the case in which the potential $V_{ls,l's'}^{J}$ in (2.9) has off-diagonal elements.[56] It is then most convenient to write (2.10) in matrix notation suppressing the indices; thus

$$-(d^2/dr^2)\Psi_J+V^J\Psi_J+[L(L+1)/r^2]\Psi_J=k^2\Psi_J, \quad (9.1)$$

where V^J is the square matrix (2.9), L is the diagonal matrix of the l values, and Ψ_J is the square matrix $\Psi_{ls,l's'}^{J}$ of (2.6). It may be well to recall the meaning of this square matrix: Each column is a solution of (9.1), its components indicating the various angular momentum components; the columns differ from one another by their boundary conditions, e.g., by the incoming wave according to (2.8). It is more convenient to work with such a square matrix then with the individual columns.

The fact that (9.1) has equations of different angular momenta coupled together leads to certain complications owing to the different behavior at $r=0$ of the solutions belonging to different l values. We want to introduce a regular solution $\Phi_J(k,r)$ which would be the generalization of $\varphi_l(k,r)$. However, the boundary condition (3.3) cannot be generalized in any simple way.[58] It is easier to write down directly the matrix integral equation that is to replace (3.7). But unless special precautions are taken or else a very strong assumption is made concerning the behavior of the off-diagonal elements of V^J, the resulting integral diverges at $r=0$. This divergence can be eliminated by adding a judicious inhomogeneity in the integral equation. We shall restrict ourselves to the case of $s=s'=1$ with tensor force coupling. The procedure is readily generalized to higher spin values.

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[55] R. G. Newton, Phys. Rev. **101**, 1588 (1956).

[56] The content of this section follows Newton and Jost,[57] and Newton.[17] The order of the matrices, however, has been changed. Equations in footnote references 17 and 57 have to be read from right to left in order to agree with those in this section.

[57] R. G. Newton and R. Jost, Nuovo cimento **1**, 590 (1955).

[58] A simple example of a square well V^J furnishes an illustration; see W. Rarita and J. Schwinger, Phys. Rev. **59**, 436 (1941). If one wants to solve the equations by series expansion, even the regular solution contains the logarithmic terms of the Fuchs theory; cf., e.g., E. L. Ince, *Ordinary Differential Equations* (Longmans, Green and Co., Ltd., New York, 1927), p. 356 ff.

If we write

$$U_J(k,r)\equiv\begin{pmatrix} k^{-J}u_{J-1}(kr) & 0 \\ 0 & k^{-J-2}u_{J+1}(kr)\end{pmatrix}, \quad (9.2)$$

$$\mathcal{G}_J(k;r,r')\equiv\begin{pmatrix} g_{J-1}(k;r,r') & 0 \\ 0 & g_{J+1}(k;r,r')\end{pmatrix}, \quad (9.3)$$

with $g_l(k;r,r')$ given by (3.6), then we can define a regular matrix solution $\Phi_J(k;r)$ of (9.1) by the integral equation

$$\Phi_J(k,r)=U_J(k,r)\left[1+(2J+1)\int_1^r dr'r'^{-1}V_T{}^J(r')\right]$$
$$+\int_0^r dr'[\mathcal{G}_J(k;r,r')V^J(r')\Phi_J(k,r')$$
$$-(2J+1)U_J(k,r)V_T{}^J(r')], \quad (9.4)$$

where

$$V_T{}^J\equiv\begin{pmatrix} 0 & 0 \\ V_{J-1,J+1}{}^J & 0\end{pmatrix}.$$

This integral equation can always be solved by successive approximations if the elements of V^J satisfy (3.1a); the matrix function $\Phi_J(k,r)$ has all the regularity and reality properties of $\varphi_l(k,r)$.

The generalization of the solution $f_l(k,r)$ is a matrix function $F_J(k,r)$ defined by the boundary condition

$$\lim_{r\to\infty}e^{ikr}F_J(k,r)=i^L, \quad (9.5)$$

or the integral equation

$$F_J(k,r)=W_J(kr)$$
$$-\int_r^\infty dr'\mathcal{G}_J(k;r,r')V^J(r')F_J(k,r') \quad (9.6)$$

with

$$W_J(kr)=\begin{pmatrix} w_{J-1}(kr) & 0 \\ 0 & w_{J+1}(kr)\end{pmatrix}.$$

Under the hypothesis (3.1b) on all elements of the potential matrix this integral equation can also always be solved by successive approximations. $F_J(k,r)$ has all the regularity properties of $f_l(k,r)$.

The generalized Jost function $F_J(k)$ is defined by the analog of (4.3)

$$F_J(k)\equiv k^L W[F_J(k,r),\Phi_J(k,r)], \quad (9.7)$$

where the Wronskian matrix[59]

$$W[F,\Phi]\equiv F^T\Phi'-F^{T\prime}\Phi$$

is defined so that it is independent of r if F and Φ both solve the same Eq. (9.1). In terms of $F_J(k)$ we have

$$\Phi_J(k,r)=\tfrac{1}{2}i[F_J(k,r)F_J{}^T(-k)$$
$$-(-)^L F_J(-k,r)F_J{}^T(k)]k^{-L-1} \quad (9.8)$$

instead of (4.1). The matrix function $F_J(k)$ has all the regularity properties of $f_l(k)$.

Comparison of the asymptotic form of (9.8) by (9.5) with (2.23) then gives us the S matrix

$$S^J(k)=F_J{}^T(k)[F_J{}^T(-k)]^{-1}. \quad (9.9)$$

This can be transformed by using the fact that because of the boundary condition

$$W[\Phi_J(k,r),\Phi_J(k,r)]=0.$$

If (9.8) is inserted in this one obtains

$$F_J(-k)F_J{}^T(k)=F_J(k)F_J{}^T(-k), \quad (9.10)$$

which shows that (9.9) can also be written

$$S^J(k)=[F_J(k)]^{-1}F_J(k), \quad (9.9')$$

at the same time verifying the symmetry of S^J. Since $F_J(k)$ has the property (4.7) it follows also that S^J is unitary. Furthermore, (9.9') implies that

$$S^J(-k)=[S^J(k)]^{-1}. \quad (9.11)$$

The relation of the physical wave function Ψ_J to Φ_J is seen by comparing (9.8) with (2.23), together with (9.5) and (9.9):

$$\Psi_J(k,r)=\Phi_J(k,r)k^{L+1}[F_J{}^T(-k)]^{-1}. \quad (9.12)$$

This is the analog of (4.8).

An integral representation for $F_J(k)$ can again be written down, but it is complicated by the extra inhomogeneities in (9.4). $F_J(k)$ being a matrix, it is not related in any direct way to the Fredholm determinant of (2.8).

The bound states can again be obtained from $F_J(k)$. This time they are those points $k=k_0$ in the lower half plane where $\det F_J(k_0)=0$. Why that is so is most easily understood by introducing an auxiliary irregular solution $I_J(k,r)$, which satisfies

$$W[I_J,\Phi_J]=1,$$
$$W[I_J,I_J]=0, \quad (9.13)$$

and which, for all fixed $r\neq 0$, is an entire function of k^2.[17] We can then express $F_J(k,r)$ in terms of $\Phi_J(k,r)$ and $I_J(k,r)$,

$$F_J(k,r)=\Phi_J(k,r)k^L F_J{}'(k)+I_J(k,r)k^{-L}F_J(k), \quad (9.14)$$

where

$$F_J{}'(k)\equiv -k^{-L}W[F_J,I_J].$$

In contrast to (9.8), (9.14) always holds in the lower half of the complex k plane, too.

Now, if $\det F_J(k_0)=0$ and $\mathrm{Im}k_0<0$, then there exists a constant vector a so that $F_J(k_0)a=0$. Equation (9.14)

[59] A superscript "T" indicates the transposed matrix. The symmetry of the potential matrix is an important assumption. By (2.17) it follows from time reversal invariance of the interaction H_I.

then shows that

$$F_J(k_0,r)a=\Phi_J(k_0,r)k_0{}^L F_J{}'(k_0)a \tag{9.15}$$

is a solution regular at the origin and exponentially decreasing at infinity; $k_0{}^2$ is thus a discrete eigenvalue and $F_J(k_0,r)a$ is the corresponding eigenfunction. Again it follows that k_0 must lie on the negative imaginary axis. Conversely, if $k_0{}^2$ is a discrete eigenvalue, then there must exist a constant vector a so that (9.15) holds and hence by (9.14)

$$I_J(k_0,r)k_0{}^{-L}F_J(k_0)a=0$$

identically in r. It then follows from (9.13) that $F_J(k_0)a=0$ and consequently $\det F_J(k_0)=0$.

The significance of the vector a is shown by (9.15). By the boundary condition (9.5) the asymptotic form of the bound-state wave function is proportional to

$$\exp(-|k_0|r)(a_1,-a_2).$$

In that sense the ratio of the components of a determines the mixture of angular momenta that forms a bound state. It is always possible that accidentally more than one mixture is bound with the same energy; that is the degenerate case. In the present instance of only two coupled angular momenta it would imply that $F_J(k_0)=0$.

It can be proved[17,57] that if $\det F_J(k_0)=0$ when $\mathrm{Im}k_0<0$, then $[F_J(k)]^{-1}$ has exactly a simple pole at $k=k_0$. That statement has no bearing on the question of degeneracy. The contrary is true for $\det F_J(k)$, which in the degenerate case has a double zero and hence its inverse, a double pole.

The point $k=0$ is somewhat complicated. For $J>1$, $\det F_J(0)=0$ implies a zero-energy bound state; for $J=1$ it does so only if $[F_J(0)]_{22}=0$ and $k^2[F_J(k)]_{12}\to 0$ as $k\to 0$. The matrix function $k^{-L}F_J(k)k^L$ is continuous at $k=0$, and the analog of (4.25) is that

$$Q_J\equiv\lim_{k\to 0}k^{2-L}[F_J(k)]^{-1}k^L \tag{9.16}$$

always exists and differs from zero if and only if $E=0$ is a discrete eigenvalue.

The argument concerning the finiteness of the number of zeros of $f_l(k)$ in the lower half-plane can be carried over directly to $F_J(k)$. Again the result is that the number of bound states for a given J is finite if all elements of V^J satisfy (3.1).

At high energies we have the analog of (4.16). For $\mathrm{Im}k\leq 0$

$$\lim_{|k|\to\infty}F_J(k)=1 \tag{9.17}$$

and consequently,

$$\lim_{k\to\pm\infty}S^J(k)=1.$$

The statements made in Secs. 4 and 5 concerning the high-energy behavior in the upper half of the complex plane under stronger assumptions on the potential carry over to the present case.

At low energies one can generalize first of all (5.15). If we define

$$2i\eta_J(k)\equiv\log\det S^J(k) \tag{9.18}$$

then comparison with (2.20) shows that η_J is the sum of the eigenphaseshifts of total angular momentum J

$$\eta_J(k)=\textstyle\sum_\alpha\delta_\alpha{}^J(k). \tag{9.18'}$$

One can then show that[57]

$$\eta_J(0)-\eta_J(\infty)=\begin{cases}\pi(n_J+\frac{1}{2}), & \text{if } J=1 \text{ and } k=0 \text{ is a resonance,}\\ \pi n_J, & \text{otherwise,}\end{cases} \tag{9.19}$$

n_J being the number of bound states of total angular momentum J (counted twice in the degenerate case); the resonant case is that in which $\det F_1(0)=0$ and $Q_1=0$ [see (9.16)].

The way in which S^J approaches its zero-energy value is found similarly as in the case of no coupling. The result is that, provided the $(2J+4)$-th absolute moments of all elements of V^J exist and they are absolutely integrable, the generalization of (5.19) is

$$S^J(k)-1=\begin{pmatrix}0(k^{2J-1}) & 0(k^{2J+1})\\ 0(k^{2J+1}) & 0(k^{2J+3})\end{pmatrix}\text{ as } k\to 0 \tag{9.20}$$

unless $\det F_J(0)=0$; in the latter case we have

$$\begin{aligned}S^J(k)-1&=\begin{pmatrix}0(k^{2J-3}) & 0(k^{2J-1})\\ 0(k^{2J-1}) & 0(k^{2J+1})\end{pmatrix},\text{ if } J>1,\\ &=\begin{pmatrix}0(k) & 0(k^3)\\ 0(k^3) & 0(k^3)\end{pmatrix},\text{ if } J=1,\end{aligned} \tag{9.20'}$$

unless we have the "resonance case."

We may now write down the complete Green's function which solves

$$\left[-\frac{d^2}{dr^2}+V^J(r)+\frac{L(L+1)}{r^2}-k^2\right]\mathfrak{G}_J(k;r,r')=-\delta(r-r'). \tag{9.21}$$

The arguments leading to its construction are the same as in Sec. 6. The result is the analog of (6.3),

$$\mathfrak{G}_J(k;r,r')=\begin{cases}(-)^J\Phi_J(k,r)k^L[F_J{}^T(-k)]^{-1}F_J{}^T(-k,r'), & r<r',\\ (-)^J F_J(-k,r)[F_J(-k)]^{-1}k^L\Phi_J{}^T(k,r'), & r>r',\end{cases} \tag{9.22}$$

or by (9.12)

$$\mathfrak{G}_J(k;r,r')=\begin{cases}(-)^J\Psi_J(k,r)F_J{}^T(-k,r'), & r<r'\\ (-)^J F_J(-k,r)\Psi_J{}^T(k,r'), & r>r'.\end{cases} \tag{9.22'}$$

The verification that this is indeed a Green's function,

i.e., that it is continuous at $r=r'$ and fulfills the matrix version of (6.2) is not completely trivial. It rests on the observation that[60]

$$F_J(k,r)F_J{}^T(-k,r)-F_J(-k,r)F_J{}^T(k,r)=0,$$
$$F_J'(k,r)F_J{}^T(-k,r)-F_J'(-k,r)F_J{}^T(k,r)=(-)^J 2ik. \tag{9.23}$$

These equations are proved by introducing an auxiliary matrix solution $\Lambda(k,r)$ of (2.10), which satisfies the boundary condition

$$\Lambda(k,r_0)=0, \quad \Lambda'(k,r_0)=1,$$

at an arbitrary point $r_0\neq 0$. Λ can be expressed in terms of $F_J(k,r)$ and $F_J(-k,r)$, the coefficients being found by evaluating the Wronskians. If we then insert the boundary condition at r_0 we obtain (9.23).

The regularity properties of $\mathfrak{G}_J$ are the same as those of $\mathfrak{G}_l$. We can again relate the S matrix to it by solving (2.8):

$$\Psi_J(k,r)=k^{L+1}U_J(k,r)+\int_0^\infty dr'\mathfrak{G}_J(k;r,r')V^J(r')U_J(k,r')k^{L+1} \tag{9.24}$$

and then inserting this solution in (2.21)

$$S^J(k)=1-2ik^{L+\frac{1}{2}}\int_0^\infty drU_J(k,r)V^J(r)U_J(k,r)k^{L+\frac{1}{2}}$$
$$-2ik^{L+\frac{1}{2}}\int_0^\infty dr\int_0^\infty dr'U_J(k,r)V^J(r)\times\mathfrak{G}_J(k;r,r')V^J(r')U_J(k,r')k^{L+\frac{1}{2}}. \tag{9.25}$$

The completeness of the eigenfunction of (9.1) is proved[17,57] by the same method as in Sec. 7 for a single equation. The result is that (7.9′) is replaced by

$$\int\Phi_J(E,r)d\mathrm{P}_J(E)\Phi_J{}^T(E,r')=\delta(r-r'), \tag{9.26}$$

where the spectral function is given by

$$\frac{d\mathrm{P}_J(E)}{dE}=\begin{cases}\dfrac{2\mu}{\pi\hbar^2}k^{L+\frac{1}{2}}[F_J(k)F_J{}^T(-k)]^{-1}k^{L+\frac{1}{2}}, & E>0,\\ \sum_n C_n\delta(E-E_n), & E\leq 0,\end{cases} \tag{9.27}$$

with $\mathrm{P}_J(-\infty)=0$. $\mathrm{P}_J(E)$ is a real, symmetric, positive semidefinite matrix function of E. The matrices C_n are real symmetric, positive semidefinite, and in general singular, with the property

$$C_n=\int_0^\infty drC_n\Phi_J{}^{(n)T}(r)\Phi_J{}^{(n)}(r)C_n, \tag{9.28}$$

where

$$\Phi_J{}^{(n)}(r)\equiv\Phi_J(-i\kappa_n,r).$$

We can always write

$$C_n=\alpha_n{}^2B_n,$$

where α_n is a real number and B_n, a real symmetric projection[61]:

$$B_n=b_n\times b_n$$

in terms of the "vector"

$$b_n=(1+\beta_n{}^2)^{-\frac{1}{2}}(1,\beta_n).$$

We also define a vector

$$\psi_J{}^{(n)}(r)\equiv\alpha_n(1+\beta_n{}^2)^{-\frac{1}{2}}\times[\Phi_{J11}{}^{(n)}(r)+\beta_n\Phi_{J12}{}^{(n)}(r),\Phi_{J21}{}^{(n)}(r)+\beta_n\Phi_{J22}{}^{(n)}(r)]$$

with the property

$$\int_0^\infty dr|\psi_J{}^{(n)}(r)|^2=1,$$

which follows from (9.28). With these definitions we have

$$\Phi_J{}^{(n)}(r)C_n\Phi_J{}^{(n)T}(r')=\psi_J{}^{(n)}(r)\times\psi_J{}^{(n)}(r').$$

The completeness (9.26) thus can also be written in terms of the physical wave function and normalized bound-state wave functions:

$$\frac{2}{\pi}\int_0^\infty dk\Psi_J(k,r)\Psi_J{}^\dagger(k,r')+\sum_n\psi_J{}^{(n)}(r)\times\psi_J{}^{(n)}(r')=\delta(r-r'). \tag{9.26′}$$

Similarly, for the complete Green's function

$$\mathfrak{G}_J(E;r,r')=\frac{\hbar^2}{2\mu}\int\frac{\Phi_J(E',r)d\mathrm{P}_J(E')\Phi_J{}^T(E',r)}{E-E'}, \tag{9.29}$$

or

$$\mathfrak{G}_J(k;r,r')=\frac{1}{\pi}\int_{-\infty}^\infty\frac{dk'}{k'}\frac{\Psi_J(k',r)\Psi_J{}^\dagger(k',r')}{k-k'}+\sum\frac{\psi_J{}^{(n)}(r)\times\psi_J{}^{(n)}(r')}{k^2+\kappa_n{}^2}. \tag{9.29′}$$

The Gel'fand Levitan equations can be generalized to the case with coupling in a straight forward manner.[57] The result is that (8.5)–(8.7), and (8.11) are replaced by

$$\Phi_J(k,r)=\Phi_J{}^{(1)}(k,r)+\int_0^\infty dr'K_J(r,r')\Phi_J{}^{(1)}(k,r'), \tag{9.30}$$

$$K_J(r,r')=\int\Phi_J(k,r)\times d[\mathrm{P}_J{}^{(1)}(E)-\mathrm{P}_J(E)]\Phi_J{}^{(1)T}(k,r'), \tag{9.31}$$

[60] Notice the position of the transposed functions. These are *not* Wronskians and their constancy is not a simple consequence of the differential equation.

[61] The cross denotes a direct product: $B_{ij}=b_ib_j$.

$$\frac{\partial^2}{\partial r^2}K_J(r,r')-\left[V^J(r)+\frac{L(L+1)}{r^2}\right]K_J(r,r')$$

$$=\frac{\partial^2}{\partial r'^2}K_J(r,r')-K_J(r,r')\left[V^{(1)J}(r')+\frac{L(L+1)}{r'^2}\right], \quad (9.32)$$

$$g_J(r,r')=\int \Phi_J{}^{(1)}(k,r)$$

$$\times d[\mathrm{P}_J{}^{(1)}(E)-\mathrm{P}_J(E)]\Phi_J{}^{(1)T}(k,r'), \quad (9.33)$$

while (8.8) to (8.10) retain the same form as before.

The potential matrix V^J is thus determined from the spectral function $\mathrm{P}_J(E)$ in the same manner as in the case of no coupling. However, it is now no longer so simple to infer the generalized Jost function $F_J(k)$ and thus $\mathrm{P}_J(E)$ from $S^J(k)$ and the bound states. The procedure leading to (5.21) cannot be generalized, the logarithm of a matrix not being well defined.[62] The problem was solved by Newton and Jost[57] with the result that, in contrast to the case of no coupling, not all matrix functions $S^J(k)$ admit of a splitup (9.9′) with $F_J(k')$ having all the required properties. No simple way is known to determine whether or not a given $S^J(k)$ leads to an $F_J(k)$, except to solve the integral equation of footnote reference 57 in order to find F_J.

10. EXAMPLES

(a) Square Well

In the simple case of a square well[63] one readily finds that the Jost function is

$$f_l(k)=(k/K)^l[w_l(kr_0)u_l'(Kr_0)-(k/K)u_l(Kr_0)w_l'(kr_0)], \quad (10.1)$$

where r_0 is the radius of the potential of strength V_0, $K^2=k^2-V_0$, and the prime indicates differentiation with respect to the argument of the function. In the case $l=0$ we have

$$f_0(k)=(r_0K)^{-1}e^{-ikr_0}\sin(Kr_0)g(-ikr_0),$$

where, with

$$z=-ikr_0, \quad z_0{}^2=-r_0{}^2V_0, \quad \zeta^2=z_0{}^2-z^2\equiv(\xi^2+i\eta)^2,$$

we write

$$g(z)=\zeta\cot\zeta-z.$$

The zeros of $f_0(k)$ are found from those of $g(z)$. The real roots with $z<z_0$ are determined by the intersection of the two curves

$$z=\xi\cot\xi, \quad z=(z_0{}^2-\xi^2)^{\frac{1}{2}},$$

shown in Fig. 1 with some intersections for $z_0{}^2>0$, i.e., an attractive potential. An intersection for negative z means a negative imaginary root of $f_0(k)$ and hence, a bound state. Such a root evidently exists whenever $z_0>\frac{1}{2}\pi$. When $1<z_0<\frac{1}{2}\pi$, then there is an intersection for positive z, i.e., a positive imaginary root of $f_0(k)$. We then have a "virtual bound state." When $z_0<1$ then we must replace ξ by $i\eta$ and the curves become

$$z=\eta\coth\eta, \quad z=(z_0{}^2+\eta^2)^{\frac{1}{2}}.$$

The intersection keeps moving up and there is always a virtual bound state.

For $z_0{}^2<0$ (i.e., a repulsive potential), there is obviously no intersection and we never have a virtual bound state.

The complex zeros of $f_0(k)$ are obtained from those roots of

$$H(z)\equiv g(z)g(-z)=\csc^2\zeta(\zeta-z_0\sin\zeta)(\zeta+z_0\sin\zeta)\equiv h(\zeta),$$

which lie in the right half of the complex z plane. A zero ζ_0 of $h(\zeta)$ must satisfy the equations

$$\xi_0\cot\xi_0=\eta_0\coth\eta_0$$
$$\xi_0=\pm z_0\sin\xi_0\cosh\eta_0$$

if the potential is attractive, or

$$\xi_0\tan\xi_0=-\eta_0\tanh\eta_0$$
$$\eta_0=\pm z_0\sin\xi_0\cosh\eta_0$$

if it is repulsive. They can be shown to have infinitely many solutions.[64]

(b) Zero-Range Potential

The case of a potential of zero range is included here only for the sake of cautioning the unwary. If the potential vanishes identically for $r>R$ then the wave function in the outside region is determined by assigning it at $r=R$ a given logarithmic derivative c which becomes less and less energy dependent the shorter the potential range R. In the limit as $R\to 0$, then, the

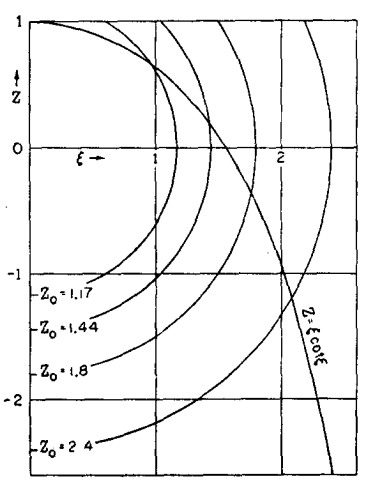

FIG. 1. Bound and virtual bound states in a square well; $z=-ikr_0$, $z_0{}^2=-r_0{}^2V_0$. The z coordinate of the intersection of the curve $z=\xi\cot\xi$ with the circle $z^2+\xi^2=z_0{}^2$ gives the energy of the bound state, if negative, or of the virtual bound state, if positive.

[62] It is not known whether $F_J(k)$ is diagonalizable or, if it is, whether its eigenvalues and diagonalizing matrix separately are analytic functions.

[63] This case was treated in great detail by Nussenzweig.[64] The procedure below is similar to his.

[64] H. M. Nussenzweig, Nuclear Phys. 3, 499 (1959).

potential is replaced by the boundary condition[65]

$$\lim_{r\to 0}\varphi'(k,r)/\varphi(k,r)=c,$$

while (3.3) is discarded. The function $f(k,r)$ is in this case simply the free function e^{-ikr} and from (4.3) [Eq. (4.3′) no longer holds],

$$f(k)=c+ik.$$

This function vanishes at $k=ic$ so that if c is negative, then there is a bound state of energy $-\hbar^2c^2/2\mu$, and if c is positive, then there is a virtual bound state. Notice that (4.16) is now no longer true.

The S matrix is

$$S(k)=(c+ik)/(c-ik), \tag{10.2}$$

so that $S(\infty)=-1$. The Levinson theorem (5.15) is also violated since now

$$\delta(0)-\delta(\infty)=\pm\tfrac{1}{2}\pi. \tag{10.3}$$

depending on the sign of c. The explanation[66] of this fact is that the limit of zero range is not uniform in k, as can be seen explicitly by writing

$$\tan\delta=(k\cot kR-c)/(k+c\cot kR).$$

If we let $k\to\infty$ then we know that for fixed R, c approaches its free value $k\cot kR$, and hence $\tan\delta\to 0$; we may subsequently let $R\to 0$ and get no change. But if we let $R\to 0$ with c fixed, we get

$$\tan\delta=k/c$$

and c is independent of k. If we now let $k\to\infty$ we get the anomalous value $\tan\delta=\infty$.

(c) Repulsive Core

If the potential is positive infinite for $r<R_c$, then the boundary condition (3.3) is replaced by

$$\varphi_l(k,R_c)=0,$$
$$\varphi_l'(k,R_c)=1,$$

for each l. The solution $f_l(k,r)$ is completely unaware of the core for $r>R_c$. The analyticity properties are thus quite unchanged. The Jost function is given by (4.3), but instead of (4.3′), we get

$$f_l(k)=k^l f_l(k,R_c),$$

and hence by (3.17), as $|k|\to\infty$ in the lower half-plane or on the real axis,

$$f_l(k)=(ik)^l e^{-ikR_c}+o(k^l e^{rR_c}).$$

The S matrix is

$$S_l(k)=(-)^l[f_l(k,R_c)/f_l(-k,R_c)].$$

Thus as $|k|\to\infty$ for real k

$$\delta_l(k)\sim -kR_c+\tfrac{1}{2}\pi l+o(1).$$

In other words, the phaseshift no longer tends to a multiple of 2π at high energies, but instead keeps increasing linearly.

The S matrix elements of the first three angular momenta for a *pure* repulsive core are

$$S_0(k)=\exp(-2ikR_c),$$
$$S_1(k)=-\exp(-2ikR_c)\cdot\frac{k-iR_c^{-1}}{k+iR_c^{-1}}, \tag{10.4}$$
$$S_2(k)=\exp(-2ikR_c)\cdot\frac{(kR_c)^2-3ikR_c-3}{(kR_c)^2+3ikR_c-3}.$$

Whereas for $l=0$, S_l is an entire function, for $l\geq 1$ it has poles in the lower half-plane, i.e., on the second sheet of the Riemann surface as a function of the energy.

Although the Levinson theorem (5.15) is not true when a repulsive core is present, one can prove a similar theorem for the difference between the actual phaseshift and the pure core phaseshift for the same core radius.

(d) Exponential Potential

If the potential has the form

$$V(r)=-V_0e^{-r/a},$$

then the s wave radial equation is explicitly solvable by setting $x=e^{-r/a}$. The result is that[12,67,68]

$$f_0(k,r)=\exp[-iak\log(a^2V_0)]\times\Gamma(1+2iak)J_{2iak}(2aV_0^{\frac{1}{2}}e^{-r/2a}) \tag{10.5}$$

and the Jost function

$$f_0(k)=\exp[-iak\log(a^2V_0)]\times\Gamma(1+2iak)J_{2iak}(2aV_0^{\frac{1}{2}}). \tag{10.6}$$

The points where

$$J_{2iak}(2aV_0^{\frac{1}{2}})=0$$

determine the bound states (for $\mathrm{Im}k_0<0$) and the virtual states as well as the "resonances."[69]

The function $f_0(k)$ has infinitely many simple poles on the positive imaginary axis because of the gamma function. They occur at $k=in/2a$ for all positive integers n. There is the exceptional possibility that $E=-\hbar^2n^2/8a^2\mu$ is the energy of a bound state. Since $J_{-n}(z)=(-)^nJ_n(z)$ the Bessel function then vanishes at the same point where the gamma function has a pole. In that case $f_0(k)$ does not have a pole at $k=in/2a$;

[65] This works only for $l=0$.

[66] This remark is due to R. E. Peierls; private communication.

[67] H. A. Bethe and R. Bacher, Revs. Modern Phys. **8**, 111 (1936).

[68] S. T. Ma, Phys. Rev. **69**, 668 (1946).

[69] It follows incidentally that $J_\nu(z)$ can have no real zeros for $\mathrm{Re}\nu>0$ unless $\mathrm{Im}\nu=0$. This does not appear to be a known property of Bessel functions.

but since it still has a zero at $k=-in/2a$, the S matrix still retains its pole.

It may be expected from the structure of $f_0(k,r)$ for the pure exponential potential that the appearance of poles in $f_0(k)$ at $k=in/2a$ for positive integers n is a general feature of potentials whose asymptotic tail is proportional to $e^{-r/a}$. This has indeed been demonstrated recently by Peierls.[70]

(e) Yukawa-Type Potentials

Suppose that the potential can be written in the form

$$V(r)=V_0\int d\alpha\rho(\alpha)e^{-\alpha r}, \tag{10.7}$$

where $\rho(\alpha)=0$ for $\alpha<\mu$, $\mu>0$.[71] A special case is the Yukawa potential, obtained by setting $\rho(\alpha)=$ const. for $\alpha>\mu$. We shall examine the implications of the foregoing form of V for $l=0$ only.[12,15,26,70,72]

If we write

$$g(k,r)\equiv f_0(k,r)e^{ikr},$$

then the integral equation (3.8) becomes for the potential (10.7)

$$g(k,r)=1+(V_0/2ik)\int d\alpha\rho(\alpha)\int_0^\infty dr' \times(1-e^{-2ikr'})e^{-\alpha(r+r')}g(k,r+r'),$$

and the Jost function is

$$f_0(k)=g(k,0).$$

We solve the integral equation by iteration

$$g(k,r)=\sum_{n=0}^{\infty}g_n(k,r),$$

and easily find that

$$g_0(k,r)=1,$$

$$g_n(k,r)=V_0{}^n\int\frac{d\alpha_1}{\alpha_1}\frac{\rho(\alpha_1)}{\alpha_1+2ik}\int\frac{d\alpha_2}{\alpha_2}\frac{\rho(\alpha_2-\alpha_1)}{\alpha_2+2ik}\cdots \times\int\frac{d\alpha_n}{\alpha_n}\frac{\rho(\alpha_n-\alpha_{n-1})}{\alpha_n+2ik}e^{-\alpha_n r},\quad n\geq 1. \tag{10.8}$$

It is clear from this that in general $f_0(k,r)$ will have a branch cut along the positive imaginary axis starting at $k=\frac{1}{2}i\mu$ and running to infinity. Moreover, if we assume that $\rho(\alpha)$ is bounded

$$|\rho(\alpha)|\leq M,$$

then $f_0(k,r)$ is a regular analytic function in the entire k plane, except for the cut; at $k=\frac{1}{2}i\mu$ it has a logarithmic singularity (unless $\rho(\mu)=0$), while everywhere else on the cut it is continuous. It is readily seen from the foregoing that if k remains a finite distance away from the cut, i.e., if

$$|\mathrm{Re}k|\geq\epsilon \quad \text{if} \quad \mathrm{Im}k\geq\tfrac{1}{2}\mu-\epsilon,$$

then

$$|g_n(k,r)|\leq(McV_0/\mu)^n/n!$$

uniformly in k and r. Hence the series converges absolutely and uniformly. Similarly one establishes the existence of the derivative and thus the analyticity of $f_0(k,r)$ and $f_0(k)$ everywhere, except on the cut.

If we define functions $h_n(\alpha,k,r)$ by the recursion

$$h_0(\alpha,k,r)=e^{-\alpha r}$$

$$h_n(\alpha,k,r)=V_0\int_{\alpha+\mu}^{\infty}\frac{d\alpha'}{\alpha'}\frac{\rho(\alpha'-\alpha)}{\alpha'+2ik}h_{n-1}(\alpha',k,r),\quad n\geq 1,$$

then

$$g_n(k,r)=h_n(0,k,r),$$

and

$$h(\alpha,k,r)=\sum_{n=0}^{\infty}h_n(\alpha,k,r)$$

converges absolutely and uniformly so long as k stays at least a fixed distance away from the cut which runs from $k=\frac{1}{2}i(\alpha+\mu)$ upwards. The function $h(\alpha,k,r)$ satisfies the integral equation

$$h(\alpha,k,r)=e^{-\alpha r}+V_0\int_{\alpha+\mu}^{\infty}\frac{d\alpha'}{\alpha'}\cdot\frac{\rho(\alpha'-\alpha)}{\alpha'+2ik}h(\alpha',k,r), \tag{10.9}$$

which determines $h(\alpha,k,r)$ explicitly in terms of $h(\alpha',k,r)$ for $\alpha'\geq\alpha+\mu$. For

$$k=\tfrac{1}{2}i(\alpha+\mu)-\tfrac{1}{2}i\epsilon,$$

we find

$$h(\alpha,k,r)=\frac{V_0\rho(\mu)}{\alpha+\mu}h(\alpha+\mu,k,r)\log\left(\frac{\alpha+\mu}{\epsilon}\right)+O(1). \tag{10.10}$$

Since

$$f_0(k)=1+V_0\int_{\mu}^{\infty}\frac{d\alpha}{\alpha}\frac{\rho(\alpha)}{\alpha+2ik}h(\alpha,k,0),$$

we have

$$\lim_{|k|\to\infty}f_0(k)=1$$

everywhere in the complex plane. Consequently, the S matrix is an analytic function of k, regular in the complex plane cut along the positive imaginary axis from $k=\frac{1}{2}i\mu$ to infinity, continuous on the cut, except near the point $k=\frac{1}{2}i\mu$, where it is $O[\log(2ik+\mu)]$. Furthermore,

$$\lim_{|k|\to\infty}S_0(k)=1.$$

One may then use Cauchy's theorem to express the real

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[70] R. E. Peierls, Proc. Roy. Soc. (London) **A253**, 16 (1959).

[71] This is a very strong assumption, since it implies not only that (3.14) holds for any $a<\frac{1}{2}\mu$, but also that $V(r)$ is an analytic function of r regular in the open right half of the complex plane.

[72] For explicit extension to $l>0$, see A. Martin, Nuovo cimento **15**, 99 (1960); and D. I. Fivel and A. Klein, preprint.

part of S_0 (for real k) in terms of its imaginary part, bound state contributions, and an integral over the cut along the positive imaginary axis.[15] Because of the last contribution such a dispersion relation is not very useful.

(f) Generalized Bargmann Potentials

Suppose we are given an arbitrary potential $V^{(0)}(r)$ and the corresponding functions $\varphi_l^{(0)}(k,r)$, $f_l^{(0)}(k,r)$ and $f_l^{(0)}(k)$. This potential need not satisfy (3.1), but we take it so that, except for isolated singularities $f_l^{(0)}(k)$ possesses an analytic extension into the upper half plane. In fact $V^{(0)}(r)$ may even be the Coulomb potential; in that case (3.4) is replaced by[73]

$$\lim_{r\to\infty} \exp i[kr-\eta k^{-1}\log r]f_0^{(0)}(k,r)=i^l.$$

We want to write[74] down the potential $\Delta V(r)$ which, if added to $V^{(0)}(r)$, causes a new $S_l(k)$ that differs from the old by a finite number of poles and zeros

$$S_l(k)=S_l^{(0)}(k)R(k)/R(-k), \tag{10.11}$$

where $R(k)$ is a rational function with N simple poles at $k=\beta_n(\mathrm{Im}\beta_n>0)$ and N simple zeros at $k=\alpha_n$, and which tends to one at infinity[75]:

$$R(k)=\Pi[(k-\alpha)/(k-\beta)]. \tag{10.12}$$

Among the α's we distinguish between those in the *upper* half-plane, which we call γ, $\mathrm{Im}\gamma>0$, and those in the *lower*, which we call κ, $\mathrm{Im}\kappa<0$.

We now form the functions

$$x_\beta(k,r)\equiv(\beta^2-k^2)^{-1}W[\varphi_l^{(0)}(\beta,r),f_l^{(0)}(k,r)], \tag{10.13}$$

$$y_\beta(k,r)\equiv(\beta^2-k^2)^{-1}W[\varphi_l^{(0)}(\beta,r),\varphi_l^{(0)}(k,r)], \tag{10.14}$$

$$\begin{cases} x_{\gamma\beta}(r)\equiv x_\beta(-\gamma,r) \\ x_{\kappa\beta}(r)\equiv x_\beta(\kappa,r)-i^lC_\kappa y_\beta(\kappa,r), \end{cases} \tag{10.15}$$

where C_κ are a set of arbitrary real constants.

Notice that we can also write

$$x_\beta(k,r)=\int_0^r dr'\,\varphi_l^{(0)}(\beta,r')f_l^{(0)}(k,r') +(k^2-\beta^2)^{-1}f_l^{(0)}(k), \tag{10.16}$$

$$y_\beta(k,r)=\int_0^r dr'\,\varphi_l^{(0)}(\beta,r')\varphi_l^{(0)}(k,r'). \tag{10.17}$$

We then define N functions $K_\beta(r)$ by the N equations[76]

$$\begin{aligned} &\textstyle\sum_\beta x_{\gamma\beta}(r)K_\beta(r)=-f_l^{(0)}(-\gamma,r), \\ &\textstyle\sum_\beta x_{\kappa\beta}(r)K_\beta(r)=-f_l^{(0)}(\kappa,r)+i^lC_\kappa\varphi_l^{(0)}(\kappa,r). \end{aligned} \tag{10.18}$$

The claim is that when

$$\Delta V(r)\equiv 2\frac{d}{dr}\sum_\beta K_\beta(r)\varphi_l^{(0)}(\beta,r) \tag{10.19}$$

is added to $V^{(0)}(r)$, it produces the $S_l(k)$ of (10.11) and, furthermore, there are bound states of energies $-\hbar^2\kappa^2/2\mu$ in addition to those of $V(r)$.

A few steps of simple algebra show that the functions

$$h(k,r)\equiv f_l^{(0)}(k,r)+\textstyle\sum_\beta K_\beta(r)x_\beta(k,r), \tag{10.20}$$

$$g(k,r)\equiv \varphi_l^{(0)}(k,r)+\textstyle\sum_\beta K_\beta(r)y_\beta(k,r), \tag{10.21}$$

satisfy the differential equations

$$-h''+[l(l+1)r^{-2}+V^{(0)}+\Delta V-k^2]h =\textstyle\sum_\beta \rho_\beta(r)x_\beta(k,r), \tag{10.22}$$

$$-g''+[l(l+1)r^{-2}+V^{(0)}+\Delta V-k^2]g =\textstyle\sum_\beta \rho_\beta(r)y_\beta(k,r), \tag{10.23}$$

where

$$\rho_\beta(r)\equiv -K_\beta''+[l(l+1)r^{-2}+V^{(0)}+\Delta V-\beta^2]K_\beta. \tag{10.24}$$

Now by the definitions (10.15) and (10.18) we have

$$h(-\gamma,r)\equiv 0, \quad h(\kappa,r)\equiv i^lC_\kappa g(\kappa,r), \tag{10.25}$$

insertion of which in (10.22) implies by (10.23) that

$$\textstyle\sum_\beta x_{\alpha\beta}(r)\rho_\beta(r)=0$$

for all α. We may conclude that[76] $\rho_\beta(r)=0$ for all β. The functions h and g thus both satisfy the Schrödinger equation with the new potential $V=V^{(0)}+\Delta V$.

Next we look at the boundary values. As $r\to\infty$ it is readily seen that

$$x_\beta(k,r)\sim -\tfrac{1}{2}(-)^l(k+\beta)^{-1}f_l^{(0)}(-\beta)e^{-i(k+\beta)r},$$
$$y_\beta(\kappa,r)\sim \tfrac{1}{4}i\kappa^{-l-1}(\beta-\kappa)^{-1}f_l^{(0)}(\kappa)f_l^{(0)}(-\beta)e^{-i(\beta-\kappa)r}.$$

The equations for $K_\beta(r)$, (10.18), thus become for large r

$$\textstyle\sum_\beta(\alpha-\beta)^{-1}f_l^{(0)}(-\beta)e^{-i\beta r}K_\beta(r)=-2i^{-l},$$

from which it follows that there exists a set of N constants a_β such that

$$\lim_{r\to\infty} f_l^{(0)}(-\beta)e^{-i\beta r}K_\beta(r)=-2i^{-l}a_\beta \tag{10.26}$$

and

$$1-\textstyle\sum_\beta(\alpha-\beta)^{-1}a_\beta=0. \tag{10.27}$$

We may immediately infer that

$$R(k)=1-\textstyle\sum_\beta(k-\beta)^{-1}a_\beta, \tag{10.28}$$

[73] $\eta=\mu cZZ'\alpha/\hbar$, where μ is the reduced mass, Z and Z' are the two charges in units of the electronic charge, α is the fine structure constant "1/137," and c is the velocity of light.

[74] The treatment below is a generalization of that of W. R. Theis, Z. Naturforsch. **11a**, 889 (1956), to include bound states. One may obtain these potentials also by solving the Gel'fand Levitan equation, a procedure due to Bargmann, unpublished.

[75] We use a simplified notation such as Σ_β to indicate a sum over the β_n from 1 to N.

[76] It is clear that $\det[x_{\alpha\beta}(r)]\not\equiv 0$.

both sides being rational functions of k with the same zeros and poles and the same limit as $|k| \to \infty$.

The asymptotic behavior of the function $h(k,r)$ of (10.20) for large r is now easily seen to be

$$h(k,r) \sim i^l e^{-ikr} R(-k),$$

which proves that

$$f_l(k,r) = h(k,r)/R(-k). \tag{10.29}$$

The function $g(k,r)$ of (10.21) is a regular solution of (2.10). From (10.21), (4.1), and (10.29) we see that

$$g(k,r) = \tfrac{1}{2} i k^{-l-1} [f_l^{(0)}(-k) R(-k) f_l(k,r) - (-)^l f_l^{(0)}(k) R(k) f_l(-k,r)]. \tag{10.30}$$

It follows that $S_l(k)$ is indeed given by (10.11). Moreover, by (10.25) and (10.29),

$$f_l(\kappa,r) = i^l C_\kappa \prod \frac{\kappa+\beta}{\kappa+\alpha} g(\kappa,r), \tag{10.31}$$

both sides being regular at $r=0$ and decreasing exponentially at infinity; κ is thus indeed a bound state. Since for given zeros of $f_l(k)$ in the lower half-plane (4.5) and (4.16) define $f_l(k)$ uniquely [see (5.21′)], we may conclude from (10.11) that

$$f_l(k) = f_l^{(0)}(k) R(k), \tag{10.32}$$

and hence from (10.30) and (4.1)

$$\varphi_l(k,r) = g(k,r). \tag{10.33}$$

We can also evaluate the normalization integral of $\varphi_l(\kappa,r)$. If we use the equations between (7.3) and (7.4). we get

$$N_\kappa^2 = \int_0^\infty dr\, |\varphi_l(\kappa,r)|^2 = (i\kappa)^{-l} \frac{\prod_{\alpha \neq \kappa} (\alpha^2 + |\kappa|^2)}{\prod_\beta (\beta^2 + |\kappa|^2)} \cdot \frac{f_l^{(0)}(\kappa)}{C_\kappa}. \tag{10.34}$$

The potential ΔV can be written in a somewhat simpler form. If we solve the set of Eqs. (10.18),

$$K_\beta(r) = -\sum_\alpha [x^{-1}(r)]_{\beta\alpha} U_\alpha^{(l)}(r), \tag{10.35}$$

where

$$U_\gamma^{(l)}(r) \equiv f_l^{(0)}(-\gamma, r)$$
$$U_\kappa^{(l)}(r) \equiv f_l^{(0)}(\kappa,r) - i^l C_\kappa \varphi_l^{(0)}(\kappa,r), \tag{10.36}$$

then we can write (10.19),

$$\Delta V(r) = -2(d^2/dr^2) \log \det[x_{\alpha\beta}(r)], \tag{10.37}$$

since it follows from (10.16) and (10.17) that

$$U_\alpha^{(l)}(r)\, \varphi_l^{(0)}(\beta,r) = (d/dr) x_{\alpha\beta}(r).$$

To summarize then, the potential $V = V^{(0)} + \Delta V$, where ΔV is given by (10.37), produces the functions $\varphi_l(k,r)$ and $f_l(k,r)$ given by (10.33) and (10.29), bound states of energy $\hbar^2\kappa^2/2\mu$ with wave functions $\varphi_l(\kappa,r)$ whose normalization is given by (10.34), and the S matrix element (10.11), or

$$S_l(k) = S_l^{(0)}(k) \prod \frac{k-\gamma}{k+\gamma} \cdot \frac{k+\beta}{k-\beta} \cdot \frac{k-\kappa}{k+\kappa}. \tag{10.11′}$$

We are free to choose a γ equal to a $-\kappa$. In that case S_l contains no pole and no zero because of the bound state. The potential ΔV is real if we choose the γ's and β's either purely imaginary or else in pairs symmetric with respect to the imaginary axis, and the κ's purely imaginary. The S_l of (10.11) is then unitary (if $S_l^{(0)}$ is). But one may also relax these requirements and make ΔV complex as an "optical" potential in order to simulate absorption.

If we choose $V^{(0)} \equiv 0$ then we get the Bargmann potentials,[77] which lead to a rational $S_l(k)$. They are often very useful for the construction of simple models. A potential which leads to a rational $S_l(k)$ for one $l = l_0$ will in general not lead to a rational $S_l(k)$ for $l \neq l_0$. Since for $l=0$ the functions that enter in $V(r)$ are all exponentials (multiplied by sines and cosines if we choose complex β's and γ's), the Bargmann potentials for the S-wave have in general exponential tails.[78] This shows that an exponential asymptotic form of the potential does not *necessarily* lead to infinitely many poles of S_l in the upper half-plane, although it does in general.[79]

If $l \neq 0$ then the functions entering the Bargmann potentials are spherical Bessel functions and thus they contain inverse powers of r. As a result, they generally have asymptotic tails r^{-n}, where $n \geq 3$. It has been shown[80] that a sufficient condition for a Bargmann potential to have an exponential tail is that $f_l(k) = f_l(0) + O(k^{2l})$ as $k \to 0$.

We may look at some special cases. If we take one $\gamma = ia$, one $\beta = ib$, $V^{(0)} = 0$, and $l = 0$,[77]

$$f_0(k) = (k - ia)/(k - ib),$$

or

$$k \cot\delta_0 = [ab/(b-a)] + [k^2/(b-a)],\ b \geq 0,\ a \geq 0, \tag{10.38}$$

then the effective range approximation is exact. The potential that produces this phaseshift is

$$V(r) = -\frac{8b^2}{b^2 - a^2} \left[\frac{e^{br}}{b-a} + \frac{e^{-br}}{b+a} \right]^{-2}. \tag{10.39}$$

If we set $a=0$ then we get a zero-energy resonance ($f_0(0) = 0$)

$$\tan\delta_0 = b/k;$$

the potential that produces it is

$$V(r) = -2b^2 \operatorname{sech}^2 br.$$

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[77] V. Bargmann, Revs. Modern Phys. **21**, 488 (1949).
[78] In special cases they may not, as will be seen below.
[79] See end of Sec. 10(d) and Peierls.[70]
[80] By T. Fulton (unpublished) and Newton.[55]

On the other hand, if we set $b=0$ then the phaseshift becomes

$$\tan\delta_0=-a/k.$$

Since then $\delta_0(0)-\delta_0(\infty)=-\frac{1}{2}\pi$, the Levinson theorem (5.15) is violated. The potential that produces this phaseshift is

$$V(r)=2a^2(1+ar)^{-2}.$$

Notice that in this case, which violates (3.1), the Jost function has a pole at $k=0$.

We can also make the effective range approximation exact with a bound state. A case of interest is the deuteron. The phaseshift has the form (10.38) with a replaced by κ, the binding energy being $\hbar^2\kappa^2/2\mu$. The potentials that produce that phaseshift and bound state are[81]

$$V_c(r)=-4\kappa\frac{d}{dr}\left\{\sinh br\frac{g_c(\kappa,r)}{g_c(\kappa+b,r)-g_c(\kappa-b,r)}\right\}, \quad (10.40)$$

where

$$g_c(k,r)=k^{-1}[e^{-kr}+c\sinh kr].$$

The normalized bound state wave function is

$$\phi(r)=2\left(\frac{c\kappa}{b^2-\kappa^2}\right)^{\frac{1}{2}}\frac{\sinh br}{g_c(\kappa+b,r)-g_c(\kappa-b,r)}. \quad (10.41)$$

The potentials (10.40) have asymptotic tails proportional to $e^{-2\kappa r}$, except when $c=-4$, in which case it decreases more rapidly.[82]

An amusing case is the one for which $S_0(k)\equiv 1$, i.e., which causes no s wave scattering whatever, at any energy, but which causes a bound state of zero energy. The potentials that do that are[77,83]

$$V(r)=-6(d/dr)[r^2/(c^2+r^3)].$$

The normalized bound state wave function[84] is

$$\phi(r)=\sqrt{3}cr/(c^2+r^3),$$

while

$$f_0(k,r)=e^{-ikr}-[3rk^{-2}/(c^2+r^3)][ikre^{-ikr}+e^{-ikr}-1].$$

The Levinson theorem (5.15) is again not fulfilled. One can similarly find the potential for which

$$f_0(k)=1+\kappa^2/k^2,$$

and which therefore has a bound state of binding energy $\hbar^2\kappa^2/2\mu$, but which causes no s scattering. This potential, however, has infinitely many singularities on the real axis.[83]

We can also use the preceding procedure to write down the potentials with a hard core or a Coulomb contribution but whose S matrix differs, for one l value, from that for a *pure* hard core or pure Coulomb field by a rational factor. The construction of such examples is left as an exercise to the reader.

The Bargmann potentials have been generalized by Fulton and Newton[85] to the case with coupling between two angular momenta. The resulting potentials constitute the only tensor forces for which the Schrödinger equation is known to have a solution in closed form. They have been applied to the case of low-energy neutron-proton scattering.[86]

[81] R. G. Newton, Phys. Rev. **105**, 763 (1957).

[82] It is a general property of the potentials producing a given phaseshift and given bound states of smallest binding energy $\hbar^2K_1^2/2\mu$ and largest binding energy $\hbar^2K_2^2/2\mu$ that, if one of them decreases asymptotically more rapidly than $\exp(-2K_2r)$ then it is the only one with that property, and if one of them decreases less rapidly than $\exp(-2K_1r)$ then they all do; cf. Newton.[55]

[83] H. E. Moses and S. F. Tuan, Nuovo cimento **13**, 197 (1959).

[84] This shows that when (3.1) is violated then there can be a bound state of $l=0$ with zero binding energy; when (3.1) is satisfied, that is impossible.

[85] T. Fulton and R. G. Newton, Nuovo cimento **3**, 677 (1956).

[86] R. G. Newton and T. Fulton, Phys. Rev. **107**, 1103 (1957).